

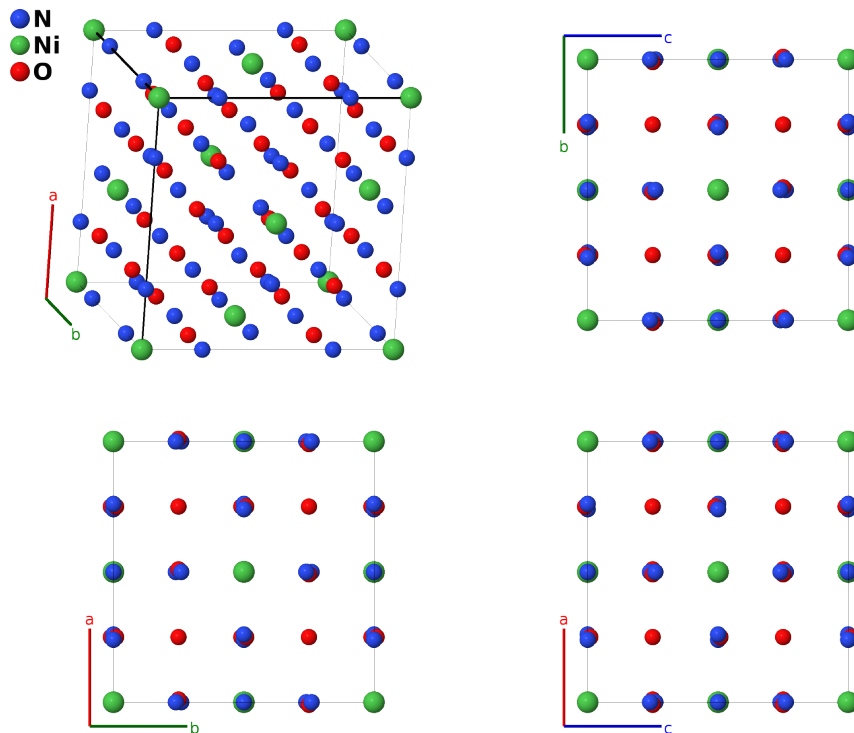
$H6_4$ $[\text{Ni}(\text{NO}_3)_2(\text{NH}_3)_6]$ Structure (*Obsolete*): A2B6CD6_cP60_205_c_d_a_d-001

This structure originally had the label A2B6CD6_cP60_205_c_d_a_d. Calls to that address will be redirected here.

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<https://aflow.org/p/GED2>

https://aflow.org/p/A2B6CD6_cP60_205_c_d_a_d-001



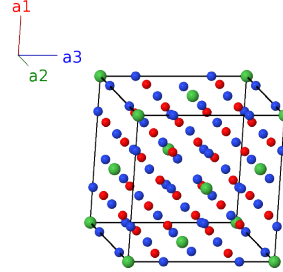
Prototype	$\text{N}_2(\text{NH}_3)_6\text{NiO}_6$
AFLOW prototype label	A2B6CD6_cP60_205_c_d_a_d-001
<i>Strukturbericht</i> designation	$H6_4$
ICSD	none
Pearson symbol	cP60
Space group number	205
Space group symbol	$Pa\bar{3}$
AFLOW prototype command	<code>aflow --proto=A2B6CD6_cP60_205_c_d_a_d-001</code> <code>--params=$a, x_2, x_3, y_3, z_3, x_4, y_4, z_4$</code>

- (Wyckoff, 1922) determined this approximate structure. In his paper, non-zero coordinates were $x_2 = 1/4$ for the nitrogen (8c) atoms, $x_3 = v$, “where v is somewhat less than 0.25,” for the NH_3 (24d) molecules, and $x_4 = y_4 = 1/4$, $z_4 = v'$, where v' “should not deviate far from 0.” If we take these coordinates as written the space group becomes $Fm\bar{3}m$ #225 rather than Wyckoff’s $Pa\bar{3}$ #205, so we adjusted v and v' slightly to put the system in his space group.

- (Ewald, 1931) gave this the *Strukturbericht* designation $H61$, or $H6_1$ in later notation. (Hermann, 1937) moved it to $I1_4$ in their “list of type descriptions,” but no other volume of *Strukturbericht* refers to it at all. Accordingly, we will designate this structure by its original label.
- This structure is an idealized approximation to the true structure of $\text{Ni}(\text{NO}_3)_2(\text{NH}_3)_6$. (Bigoli, 1971) showed that the correct structure is trigonal, with space group $P\bar{1} \#2$.

Simple Cubic primitive vectors

$$\begin{aligned}\mathbf{a}_1 &= a \hat{\mathbf{x}} \\ \mathbf{a}_2 &= a \hat{\mathbf{y}} \\ \mathbf{a}_3 &= a \hat{\mathbf{z}}\end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
\mathbf{B}_1	$= 0$	$=$	0	(4a)	Ni I
\mathbf{B}_2	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{z}}$	(4a)	Ni I
\mathbf{B}_3	$= \frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{y}} + \frac{1}{2} a \hat{\mathbf{z}}$	(4a)	Ni I
\mathbf{B}_4	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}}$	(4a)	Ni I
\mathbf{B}_5	$= x_2 \mathbf{a}_1 + x_2 \mathbf{a}_2 + x_2 \mathbf{a}_3$	$=$	$ax_2 \hat{\mathbf{x}} + ax_2 \hat{\mathbf{y}} + ax_2 \hat{\mathbf{z}}$	(8c)	N I
\mathbf{B}_6	$= -\left(x_2 - \frac{1}{2}\right) \mathbf{a}_1 - x_2 \mathbf{a}_2 + \left(x_2 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a\left(x_2 - \frac{1}{2}\right) \hat{\mathbf{x}} - ax_2 \hat{\mathbf{y}} + a\left(x_2 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(8c)	N I
\mathbf{B}_7	$= -x_2 \mathbf{a}_1 + \left(x_2 + \frac{1}{2}\right) \mathbf{a}_2 - \left(x_2 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-ax_2 \hat{\mathbf{x}} + a\left(x_2 + \frac{1}{2}\right) \hat{\mathbf{y}} - a\left(x_2 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(8c)	N I
\mathbf{B}_8	$= \left(x_2 + \frac{1}{2}\right) \mathbf{a}_1 - \left(x_2 - \frac{1}{2}\right) \mathbf{a}_2 - x_2 \mathbf{a}_3$	$=$	$a\left(x_2 + \frac{1}{2}\right) \hat{\mathbf{x}} - a\left(x_2 - \frac{1}{2}\right) \hat{\mathbf{y}} - ax_2 \hat{\mathbf{z}}$	(8c)	N I
\mathbf{B}_9	$= -x_2 \mathbf{a}_1 - x_2 \mathbf{a}_2 - x_2 \mathbf{a}_3$	$=$	$-ax_2 \hat{\mathbf{x}} - ax_2 \hat{\mathbf{y}} - ax_2 \hat{\mathbf{z}}$	(8c)	N I
\mathbf{B}_{10}	$= \left(x_2 + \frac{1}{2}\right) \mathbf{a}_1 + x_2 \mathbf{a}_2 - \left(x_2 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$a\left(x_2 + \frac{1}{2}\right) \hat{\mathbf{x}} + ax_2 \hat{\mathbf{y}} - a\left(x_2 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(8c)	N I
\mathbf{B}_{11}	$= x_2 \mathbf{a}_1 - \left(x_2 - \frac{1}{2}\right) \mathbf{a}_2 + \left(x_2 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$ax_2 \hat{\mathbf{x}} - a\left(x_2 - \frac{1}{2}\right) \hat{\mathbf{y}} + a\left(x_2 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(8c)	N I
\mathbf{B}_{12}	$= -\left(x_2 - \frac{1}{2}\right) \mathbf{a}_1 + \left(x_2 + \frac{1}{2}\right) \mathbf{a}_2 + x_2 \mathbf{a}_3$	$=$	$-a\left(x_2 - \frac{1}{2}\right) \hat{\mathbf{x}} + a\left(x_2 + \frac{1}{2}\right) \hat{\mathbf{y}} + ax_2 \hat{\mathbf{z}}$	(8c)	N I
\mathbf{B}_{13}	$= x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$ax_3 \hat{\mathbf{x}} + ay_3 \hat{\mathbf{y}} + az_3 \hat{\mathbf{z}}$	(24d)	NH I
\mathbf{B}_{14}	$= -\left(x_3 - \frac{1}{2}\right) \mathbf{a}_1 - y_3 \mathbf{a}_2 + \left(z_3 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a\left(x_3 - \frac{1}{2}\right) \hat{\mathbf{x}} - ay_3 \hat{\mathbf{y}} + a\left(z_3 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(24d)	NH I
\mathbf{B}_{15}	$= -x_3 \mathbf{a}_1 + \left(y_3 + \frac{1}{2}\right) \mathbf{a}_2 - \left(z_3 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-ax_3 \hat{\mathbf{x}} + a\left(y_3 + \frac{1}{2}\right) \hat{\mathbf{y}} - a\left(z_3 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(24d)	NH I
\mathbf{B}_{16}	$= \left(x_3 + \frac{1}{2}\right) \mathbf{a}_1 - \left(y_3 - \frac{1}{2}\right) \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$a\left(x_3 + \frac{1}{2}\right) \hat{\mathbf{x}} - a\left(y_3 - \frac{1}{2}\right) \hat{\mathbf{y}} - az_3 \hat{\mathbf{z}}$	(24d)	NH I
\mathbf{B}_{17}	$= z_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + y_3 \mathbf{a}_3$	$=$	$az_3 \hat{\mathbf{x}} + ax_3 \hat{\mathbf{y}} + ay_3 \hat{\mathbf{z}}$	(24d)	NH I
\mathbf{B}_{18}	$= \left(z_3 + \frac{1}{2}\right) \mathbf{a}_1 - \left(x_3 - \frac{1}{2}\right) \mathbf{a}_2 - y_3 \mathbf{a}_3$	$=$	$a\left(z_3 + \frac{1}{2}\right) \hat{\mathbf{x}} - a\left(x_3 - \frac{1}{2}\right) \hat{\mathbf{y}} - ay_3 \hat{\mathbf{z}}$	(24d)	NH I
\mathbf{B}_{19}	$= -\left(z_3 - \frac{1}{2}\right) \mathbf{a}_1 - x_3 \mathbf{a}_2 + \left(y_3 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a\left(z_3 - \frac{1}{2}\right) \hat{\mathbf{x}} - ax_3 \hat{\mathbf{y}} + a\left(y_3 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(24d)	NH I

$$\begin{aligned}
\mathbf{B}_{52} &= -\left(x_4 - \frac{1}{2}\right) \mathbf{a}_1 + \left(y_4 + \frac{1}{2}\right) \mathbf{a}_2 + z_4 \mathbf{a}_3 = -a\left(x_4 - \frac{1}{2}\right) \hat{\mathbf{x}} + a\left(y_4 + \frac{1}{2}\right) \hat{\mathbf{y}} + az_4 \hat{\mathbf{z}} & (24d) & \text{O I} \\
\mathbf{B}_{53} &= -z_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 - y_4 \mathbf{a}_3 = -az_4 \hat{\mathbf{x}} - ax_4 \hat{\mathbf{y}} - ay_4 \hat{\mathbf{z}} & (24d) & \text{O I} \\
\mathbf{B}_{54} &= -\left(z_4 - \frac{1}{2}\right) \mathbf{a}_1 + \left(x_4 + \frac{1}{2}\right) \mathbf{a}_2 + y_4 \mathbf{a}_3 = -a\left(z_4 - \frac{1}{2}\right) \hat{\mathbf{x}} + a\left(x_4 + \frac{1}{2}\right) \hat{\mathbf{y}} + ay_4 \hat{\mathbf{z}} & (24d) & \text{O I} \\
\mathbf{B}_{55} &= \left(z_4 + \frac{1}{2}\right) \mathbf{a}_1 + x_4 \mathbf{a}_2 - \left(y_4 - \frac{1}{2}\right) \mathbf{a}_3 = a\left(z_4 + \frac{1}{2}\right) \hat{\mathbf{x}} + ax_4 \hat{\mathbf{y}} - a\left(y_4 - \frac{1}{2}\right) \hat{\mathbf{z}} & (24d) & \text{O I} \\
\mathbf{B}_{56} &= z_4 \mathbf{a}_1 - \left(x_4 - \frac{1}{2}\right) \mathbf{a}_2 + \left(y_4 + \frac{1}{2}\right) \mathbf{a}_3 = az_4 \hat{\mathbf{x}} - a\left(x_4 - \frac{1}{2}\right) \hat{\mathbf{y}} + a\left(y_4 + \frac{1}{2}\right) \hat{\mathbf{z}} & (24d) & \text{O I} \\
\mathbf{B}_{57} &= -y_4 \mathbf{a}_1 - z_4 \mathbf{a}_2 - x_4 \mathbf{a}_3 = -ay_4 \hat{\mathbf{x}} - az_4 \hat{\mathbf{y}} - ax_4 \hat{\mathbf{z}} & (24d) & \text{O I} \\
\mathbf{B}_{58} &= y_4 \mathbf{a}_1 - \left(z_4 - \frac{1}{2}\right) \mathbf{a}_2 + \left(x_4 + \frac{1}{2}\right) \mathbf{a}_3 = ay_4 \hat{\mathbf{x}} - a\left(z_4 - \frac{1}{2}\right) \hat{\mathbf{y}} + a\left(x_4 + \frac{1}{2}\right) \hat{\mathbf{z}} & (24d) & \text{O I} \\
\mathbf{B}_{59} &= -\left(y_4 - \frac{1}{2}\right) \mathbf{a}_1 + \left(z_4 + \frac{1}{2}\right) \mathbf{a}_2 + x_4 \mathbf{a}_3 = -a\left(y_4 - \frac{1}{2}\right) \hat{\mathbf{x}} + a\left(z_4 + \frac{1}{2}\right) \hat{\mathbf{y}} + ax_4 \hat{\mathbf{z}} & (24d) & \text{O I} \\
\mathbf{B}_{60} &= \left(y_4 + \frac{1}{2}\right) \mathbf{a}_1 + z_4 \mathbf{a}_2 - \left(x_4 - \frac{1}{2}\right) \mathbf{a}_3 = a\left(y_4 + \frac{1}{2}\right) \hat{\mathbf{x}} + az_4 \hat{\mathbf{y}} - a\left(x_4 - \frac{1}{2}\right) \hat{\mathbf{z}} & (24d) & \text{O I}
\end{aligned}$$

References

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