

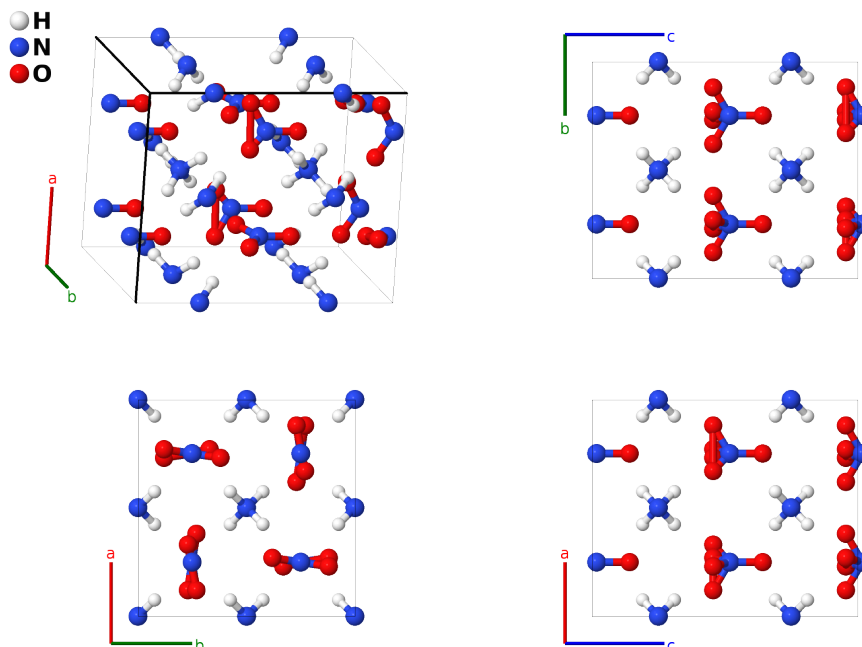
Gwihabaite (NH₄NO₃ V) Structure: A4B2C3_tP72_77_8d_ab2c2d_6d-001

This structure originally had the label A4B2C3_tP72_77_8d_ab2c2d_6d. Calls to that address will be redirected here.

Cite this page as: D. Hicks, M. J. Mehl, M. Esters, C. Oses, O. Levy, G. L. W. Hart, C. Toher, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 3*, Comput. Mater. Sci. **199**, 110450 (2021), doi: 10.1016/j.commatsci.2021.110450.

<https://aflow.org/p/JS41>

https://aflow.org/p/A4B2C3_tP72_77_8d_ab2c2d_6d-001



Prototype	H ₄ N ₂ O ₃
AFLOW prototype label	A4B2C3_tP72_77_8d_ab2c2d_6d-001
Mineral name	gwihabaite
ICSD	27453
Pearson symbol	tP72
Space group number	77
Space group symbol	P4 ₂
AFLOW prototype command	<pre>aflow --proto=A4B2C3_tP72_77_8d_ab2c2d_6d-001 --params=a, c/a, z1, z2, z3, z4, x5, y5, z5, x6, y6, z6, x7, y7, z7, x8, y8, z8, x9, y9, z9, x10, y10, z10, x11, y11, z11, x12, y12, z12, x13, y13, z13, x14, y14, z14, x15, y15, z15, x16, y16, z16, x17, y17, z17, x18, y18, z18, x19, y19, z19, x20, y20, z20</pre>

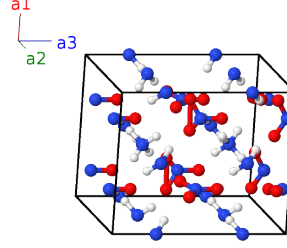
- Ammonium nitrate exists in a variety of forms, (Hermann, 1937) depending on the temperature:

Phase	Temperature °C	Strukturbericht	Page
I	125 – 170	G0 ₈	AB_cP2_221_a_b-001
II	84 – 125	G0 ₉	ABC3_tP10_100_b_a_bc-001
III	32 – 84	G0 ₁₀	ABC3_oP20_62_c_c_cd-002
IV	-18 – 32	G0 ₁₁	A4B2C3_oP18_59_ef_ab_af-001
V	< -18		A4B2C3_tP72_77_8d_ab2c2d_6d2-001 (this structure)

- Data for this structure was taken at -150°C.

Simple Tetragonal primitive vectors

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



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
\mathbf{B}_1	$= z_1 \mathbf{a}_3$	$=$	$cz_1 \hat{\mathbf{z}}$	(2a)	N I
\mathbf{B}_2	$= \left(z_1 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$c \left(z_1 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(2a)	N I
\mathbf{B}_3	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{2}a \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$	(2b)	N II
\mathbf{B}_4	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + \left(z_2 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{2}a \hat{\mathbf{y}} + c \left(z_2 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(2b)	N II
\mathbf{B}_5	$= \frac{1}{2} \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(2c)	N III
\mathbf{B}_6	$= \frac{1}{2} \mathbf{a}_1 + \left(z_3 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + c \left(z_3 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(2c)	N III
\mathbf{B}_7	$= \frac{1}{2} \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(2c)	N IV
\mathbf{B}_8	$= \frac{1}{2} \mathbf{a}_1 + \left(z_4 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + c \left(z_4 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(2c)	N IV
\mathbf{B}_9	$= x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$ax_5 \hat{\mathbf{x}} + ay_5 \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(4d)	H I
\mathbf{B}_{10}	$= -x_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$-ax_5 \hat{\mathbf{x}} - ay_5 \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(4d)	H I
\mathbf{B}_{11}	$= -y_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 + \left(z_5 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-ay_5 \hat{\mathbf{x}} + ax_5 \hat{\mathbf{y}} + c \left(z_5 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(4d)	H I
\mathbf{B}_{12}	$= y_5 \mathbf{a}_1 - x_5 \mathbf{a}_2 + \left(z_5 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$ay_5 \hat{\mathbf{x}} - ax_5 \hat{\mathbf{y}} + c \left(z_5 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(4d)	H I
\mathbf{B}_{13}	$= x_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$ax_6 \hat{\mathbf{x}} + ay_6 \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}}$	(4d)	H II
\mathbf{B}_{14}	$= -x_6 \mathbf{a}_1 - y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$-ax_6 \hat{\mathbf{x}} - ay_6 \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}}$	(4d)	H II
\mathbf{B}_{15}	$= -y_6 \mathbf{a}_1 + x_6 \mathbf{a}_2 + \left(z_6 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-ay_6 \hat{\mathbf{x}} + ax_6 \hat{\mathbf{y}} + c \left(z_6 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(4d)	H II
\mathbf{B}_{16}	$= y_6 \mathbf{a}_1 - x_6 \mathbf{a}_2 + \left(z_6 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$ay_6 \hat{\mathbf{x}} - ax_6 \hat{\mathbf{y}} + c \left(z_6 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(4d)	H II
\mathbf{B}_{17}	$= x_7 \mathbf{a}_1 + y_7 \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$ax_7 \hat{\mathbf{x}} + ay_7 \hat{\mathbf{y}} + cz_7 \hat{\mathbf{z}}$	(4d)	H III
\mathbf{B}_{18}	$= -x_7 \mathbf{a}_1 - y_7 \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$-ax_7 \hat{\mathbf{x}} - ay_7 \hat{\mathbf{y}} + cz_7 \hat{\mathbf{z}}$	(4d)	H III
\mathbf{B}_{19}	$= -y_7 \mathbf{a}_1 + x_7 \mathbf{a}_2 + \left(z_7 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-ay_7 \hat{\mathbf{x}} + ax_7 \hat{\mathbf{y}} + c \left(z_7 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(4d)	H III
\mathbf{B}_{20}	$= y_7 \mathbf{a}_1 - x_7 \mathbf{a}_2 + \left(z_7 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$ay_7 \hat{\mathbf{x}} - ax_7 \hat{\mathbf{y}} + c \left(z_7 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(4d)	H III
\mathbf{B}_{21}	$= x_8 \mathbf{a}_1 + y_8 \mathbf{a}_2 + z_8 \mathbf{a}_3$	$=$	$ax_8 \hat{\mathbf{x}} + ay_8 \hat{\mathbf{y}} + cz_8 \hat{\mathbf{z}}$	(4d)	H IV
\mathbf{B}_{22}	$= -x_8 \mathbf{a}_1 - y_8 \mathbf{a}_2 + z_8 \mathbf{a}_3$	$=$	$-ax_8 \hat{\mathbf{x}} - ay_8 \hat{\mathbf{y}} + cz_8 \hat{\mathbf{z}}$	(4d)	H IV

$$\begin{aligned}
\mathbf{B}_{64} &= y_{18} \mathbf{a}_1 - x_{18} \mathbf{a}_2 + \left(z_{18} + \frac{1}{2}\right) \mathbf{a}_3 &= ay_{18} \hat{\mathbf{x}} - ax_{18} \hat{\mathbf{y}} + c \left(z_{18} + \frac{1}{2}\right) \hat{\mathbf{z}} &(4d) & \text{O IV} \\
\mathbf{B}_{65} &= x_{19} \mathbf{a}_1 + y_{19} \mathbf{a}_2 + z_{19} \mathbf{a}_3 &= ax_{19} \hat{\mathbf{x}} + ay_{19} \hat{\mathbf{y}} + cz_{19} \hat{\mathbf{z}} &(4d) & \text{O V} \\
\mathbf{B}_{66} &= -x_{19} \mathbf{a}_1 - y_{19} \mathbf{a}_2 + z_{19} \mathbf{a}_3 &= -ax_{19} \hat{\mathbf{x}} - ay_{19} \hat{\mathbf{y}} + cz_{19} \hat{\mathbf{z}} &(4d) & \text{O V} \\
\mathbf{B}_{67} &= -y_{19} \mathbf{a}_1 + x_{19} \mathbf{a}_2 + \left(z_{19} + \frac{1}{2}\right) \mathbf{a}_3 &= -ay_{19} \hat{\mathbf{x}} + ax_{19} \hat{\mathbf{y}} + c \left(z_{19} + \frac{1}{2}\right) \hat{\mathbf{z}} &(4d) & \text{O V} \\
\mathbf{B}_{68} &= y_{19} \mathbf{a}_1 - x_{19} \mathbf{a}_2 + \left(z_{19} + \frac{1}{2}\right) \mathbf{a}_3 &= ay_{19} \hat{\mathbf{x}} - ax_{19} \hat{\mathbf{y}} + c \left(z_{19} + \frac{1}{2}\right) \hat{\mathbf{z}} &(4d) & \text{O V} \\
\mathbf{B}_{69} &= x_{20} \mathbf{a}_1 + y_{20} \mathbf{a}_2 + z_{20} \mathbf{a}_3 &= ax_{20} \hat{\mathbf{x}} + ay_{20} \hat{\mathbf{y}} + cz_{20} \hat{\mathbf{z}} &(4d) & \text{O VI} \\
\mathbf{B}_{70} &= -x_{20} \mathbf{a}_1 - y_{20} \mathbf{a}_2 + z_{20} \mathbf{a}_3 &= -ax_{20} \hat{\mathbf{x}} - ay_{20} \hat{\mathbf{y}} + cz_{20} \hat{\mathbf{z}} &(4d) & \text{O VI} \\
\mathbf{B}_{71} &= -y_{20} \mathbf{a}_1 + x_{20} \mathbf{a}_2 + \left(z_{20} + \frac{1}{2}\right) \mathbf{a}_3 &= -ay_{20} \hat{\mathbf{x}} + ax_{20} \hat{\mathbf{y}} + c \left(z_{20} + \frac{1}{2}\right) \hat{\mathbf{z}} &(4d) & \text{O VI} \\
\mathbf{B}_{72} &= y_{20} \mathbf{a}_1 - x_{20} \mathbf{a}_2 + \left(z_{20} + \frac{1}{2}\right) \mathbf{a}_3 &= ay_{20} \hat{\mathbf{x}} - ax_{20} \hat{\mathbf{y}} + c \left(z_{20} + \frac{1}{2}\right) \hat{\mathbf{z}} &(4d) & \text{O VI}
\end{aligned}$$

References

- [1] J. L. Amorós, F. Arrese, and M. Canut, *The crystal structure of the low-temperature phase of NH_4NO_3 (V) at -150°C* , Z. Kristallogr. **117**, 92–107 (1962), doi:10.1524/zkri.1962.117.2-3.92.
- [2] C. Hermann, O. Lohrmann, and H. Philipp, eds., *Strukturbericht Band II 1928-1932* (Akademische Verlagsgesellschaft M. B. H., Leipzig, 1937).

Found in

- [1] R. T. Downs and M. Hall-Wallace, *The American Mineralogist Crystal Structure Database*, Am. Mineral. **88**, 247–250 (2003).