

Gwihabaite (NH₄NO₃ V) Structure: A4B2C3_tP72_77_8d_ab2c2d_6d-001

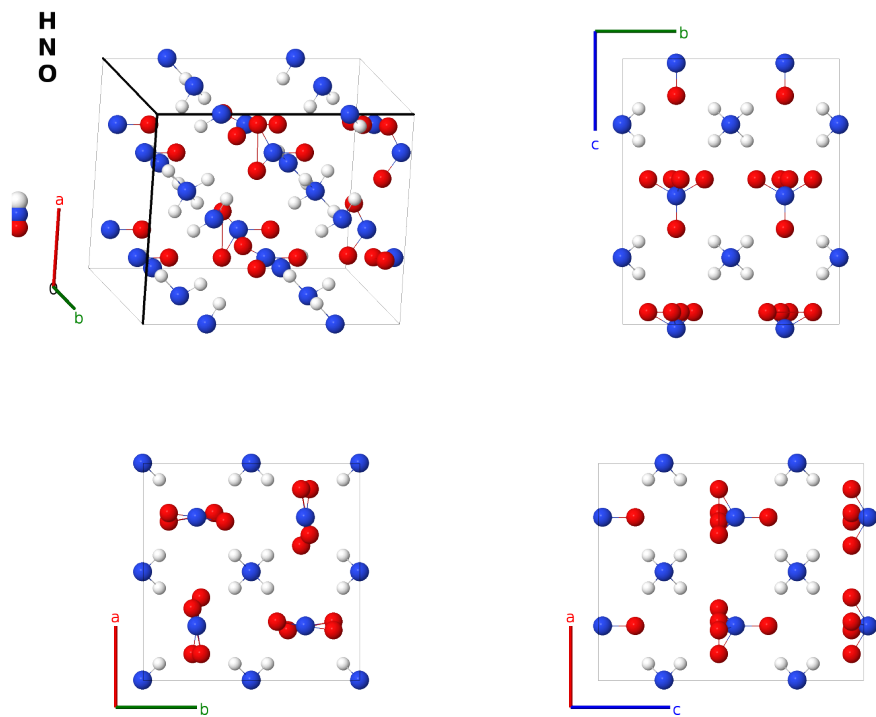
This structure previously used the label(s) **A4B2C3_tP72_77_8d_ab2c2d_6d**. Calls to these addresses will be redirected here.

Cite this page as:

- H. Eckert, S. Divilov, M. J. Mehl, D. Hicks, A. C. Zettel, M. Esters, X. Campilongo, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*, Comput. Mater. Sci. **240**, 112988 (2024), doi: 10.1016/j.commatsci.2024.112988.
- 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/prototype-encyclopedia/JS41>

https://aflow.org/prototype-encyclopedia/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
CCDC	1602729
Pearson symbol	tP72
Space group number	77
Space group symbol	P4 ₂

AFLOW prototype command `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`

- 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)

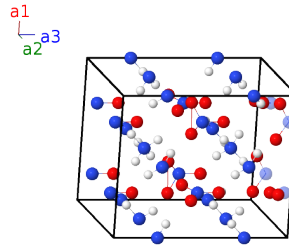
- Data for this structure was taken at -150°C.

Simple Tetragonal primitive vectors

$$\mathbf{a}_1 = a \hat{\mathbf{x}}$$

$$\mathbf{a}_2 = a \hat{\mathbf{y}}$$

$$\mathbf{a}_3 = c \hat{\mathbf{z}}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= z_1 \mathbf{a}_3$	$=$	$c z_1 \hat{\mathbf{z}}$	(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
$\mathbf{B}_3$	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} + c z_2 \hat{\mathbf{z}}$	(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
$\mathbf{B}_5$	$= \frac{1}{2} \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{y}} + c z_3 \hat{\mathbf{z}}$	(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
$\mathbf{B}_7$	$= \frac{1}{2} \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{y}} + c z_4 \hat{\mathbf{z}}$	(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
$\mathbf{B}_9$	$= x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$a x_5 \hat{\mathbf{x}} + a y_5 \hat{\mathbf{y}} + c z_5 \hat{\mathbf{z}}$	(4d)	H I
$\mathbf{B}_{10}$	$= -x_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$-a x_5 \hat{\mathbf{x}} - a y_5 \hat{\mathbf{y}} + c z_5 \hat{\mathbf{z}}$	(4d)	H I
$\mathbf{B}_{11}$	$= -y_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 + \left(z_5 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a y_5 \hat{\mathbf{x}} + a x_5 \hat{\mathbf{y}} + c \left(z_5 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(4d)	H I
$\mathbf{B}_{12}$	$= y_5 \mathbf{a}_1 - x_5 \mathbf{a}_2 + \left(z_5 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$a y_5 \hat{\mathbf{x}} - a x_5 \hat{\mathbf{y}} + c \left(z_5 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(4d)	H I
$\mathbf{B}_{13}$	$= x_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$a x_6 \hat{\mathbf{x}} + a y_6 \hat{\mathbf{y}} + c z_6 \hat{\mathbf{z}}$	(4d)	H II
$\mathbf{B}_{14}$	$= -x_6 \mathbf{a}_1 - y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$-a x_6 \hat{\mathbf{x}} - a y_6 \hat{\mathbf{y}} + c z_6 \hat{\mathbf{z}}$	(4d)	H II
$\mathbf{B}_{15}$	$= -y_6 \mathbf{a}_1 + x_6 \mathbf{a}_2 + \left(z_6 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a y_6 \hat{\mathbf{x}} + a x_6 \hat{\mathbf{y}} + c \left(z_6 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(4d)	H II
$\mathbf{B}_{16}$	$= y_6 \mathbf{a}_1 - x_6 \mathbf{a}_2 + \left(z_6 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$a y_6 \hat{\mathbf{x}} - a x_6 \hat{\mathbf{y}} + c \left(z_6 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(4d)	H II

$$\begin{aligned}
\mathbf{B}_{58} &= -x_{17} \mathbf{a}_1 - y_{17} \mathbf{a}_2 + z_{17} \mathbf{a}_3 &= -ax_{17} \hat{\mathbf{x}} - ay_{17} \hat{\mathbf{y}} + cz_{17} \hat{\mathbf{z}} &(4d) &\text{O III} \\
\mathbf{B}_{59} &= -y_{17} \mathbf{a}_1 + x_{17} \mathbf{a}_2 + \left(z_{17} + \frac{1}{2}\right) \mathbf{a}_3 &= -ay_{17} \hat{\mathbf{x}} + ax_{17} \hat{\mathbf{y}} + c \left(z_{17} + \frac{1}{2}\right) \hat{\mathbf{z}} &(4d) &\text{O III} \\
\mathbf{B}_{60} &= y_{17} \mathbf{a}_1 - x_{17} \mathbf{a}_2 + \left(z_{17} + \frac{1}{2}\right) \mathbf{a}_3 &= ay_{17} \hat{\mathbf{x}} - ax_{17} \hat{\mathbf{y}} + c \left(z_{17} + \frac{1}{2}\right) \hat{\mathbf{z}} &(4d) &\text{O III} \\
\mathbf{B}_{61} &= x_{18} \mathbf{a}_1 + y_{18} \mathbf{a}_2 + z_{18} \mathbf{a}_3 &= ax_{18} \hat{\mathbf{x}} + ay_{18} \hat{\mathbf{y}} + cz_{18} \hat{\mathbf{z}} &(4d) &\text{O IV} \\
\mathbf{B}_{62} &= -x_{18} \mathbf{a}_1 - y_{18} \mathbf{a}_2 + z_{18} \mathbf{a}_3 &= -ax_{18} \hat{\mathbf{x}} - ay_{18} \hat{\mathbf{y}} + cz_{18} \hat{\mathbf{z}} &(4d) &\text{O IV} \\
\mathbf{B}_{63} &= -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}_{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).

First cited in

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.