

NH₄NO₃ IV (*G*₀₁₁) Structure: A4B2C3_oP18_59_ef_ab_ae-001

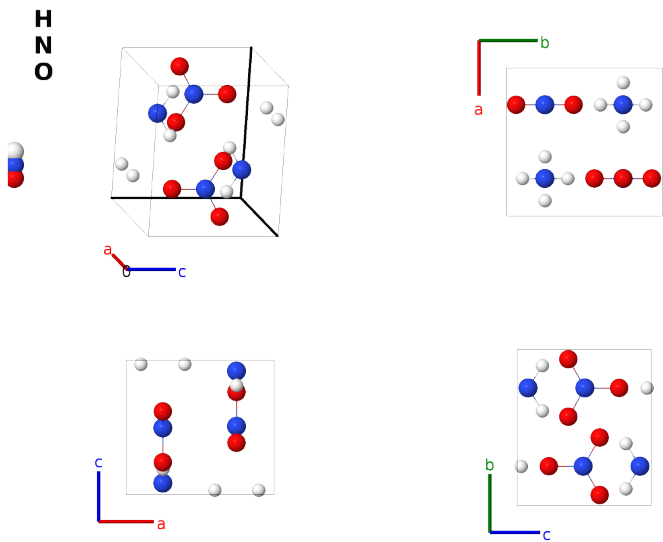
This structure previously used the label(s) **A4B2C3_oP18_59_ef_ab.af**. Calls to these addresses will be redirected here.

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. Osos, 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/NABB>

https://aflow.org/prototype-encyclopedia/A4B2C3_oP18_59_ef_ab_ae-001



Prototype	H ₄ N ₂ O ₃
AFLOW prototype label	A4B2C3_oP18_59_ef_ab_ae-001
<i>Strukturbericht</i> designation	<i>G</i> ₀₁₁
ICSD	2772
CCDC	1592576
Pearson symbol	oP18
Space group number	59
Space group symbol	<i>Pm</i> <i>mn</i>
AFLOW prototype command	<code>aflow --proto=A4B2C3_oP18_59_ef_ab_ae-001</code> <code>--params=<i>a</i>,<i>b/a</i>,<i>c/a</i>,<i>z</i>₁,<i>z</i>₂,<i>z</i>₃,<i>y</i>₄,<i>z</i>₄,<i>y</i>₅,<i>z</i>₅,<i>x</i>₆,<i>z</i>₆</code>

- 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 (this structure)
V	< -18		A4B2C3_tP72_77_8d_ab2c2d_6d2-001

- In the original reference (West, 1932) did not determine the positions of the hydrogen atoms. (Choi, 1972) found the hydrogen atoms, and found that they did not change the space group. We therefore use their structure as the prototype for $G0_{11}$.

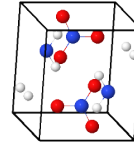
Simple Orthorhombic primitive vectors



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

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

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



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= \frac{1}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_1 \mathbf{a}_3$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} + cz_1 \hat{\mathbf{z}}$	(2a)	N I
$\mathbf{B}_2$	$= \frac{3}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_1 \mathbf{a}_3$	$=$	$\frac{3}{4}a \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} - cz_1 \hat{\mathbf{z}}$	(2a)	N I
$\mathbf{B}_3$	$= \frac{1}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$	(2a)	O I
$\mathbf{B}_4$	$= \frac{3}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_2 \mathbf{a}_3$	$=$	$\frac{3}{4}a \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} - cz_2 \hat{\mathbf{z}}$	(2a)	O I
$\mathbf{B}_5$	$= \frac{1}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(2b)	N II
$\mathbf{B}_6$	$= \frac{3}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$\frac{3}{4}a \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} - cz_3 \hat{\mathbf{z}}$	(2b)	N II
$\mathbf{B}_7$	$= \frac{1}{4} \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} + by_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(4e)	H I
$\mathbf{B}_8$	$= \frac{1}{4} \mathbf{a}_1 - (y_4 - \frac{1}{2}) \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} - b(y_4 - \frac{1}{2}) \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(4e)	H I
$\mathbf{B}_9$	$= \frac{3}{4} \mathbf{a}_1 + (y_4 + \frac{1}{2}) \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$\frac{3}{4}a \hat{\mathbf{x}} + b(y_4 + \frac{1}{2}) \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}}$	(4e)	H I
$\mathbf{B}_{10}$	$= \frac{3}{4} \mathbf{a}_1 - y_4 \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$\frac{3}{4}a \hat{\mathbf{x}} - by_4 \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}}$	(4e)	H I
$\mathbf{B}_{11}$	$= \frac{1}{4} \mathbf{a}_1 + y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} + by_5 \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(4e)	O II
$\mathbf{B}_{12}$	$= \frac{1}{4} \mathbf{a}_1 - (y_5 - \frac{1}{2}) \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} - b(y_5 - \frac{1}{2}) \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(4e)	O II
$\mathbf{B}_{13}$	$= \frac{3}{4} \mathbf{a}_1 + (y_5 + \frac{1}{2}) \mathbf{a}_2 - z_5 \mathbf{a}_3$	$=$	$\frac{3}{4}a \hat{\mathbf{x}} + b(y_5 + \frac{1}{2}) \hat{\mathbf{y}} - cz_5 \hat{\mathbf{z}}$	(4e)	O II
$\mathbf{B}_{14}$	$= \frac{3}{4} \mathbf{a}_1 - y_5 \mathbf{a}_2 - z_5 \mathbf{a}_3$	$=$	$\frac{3}{4}a \hat{\mathbf{x}} - by_5 \hat{\mathbf{y}} - cz_5 \hat{\mathbf{z}}$	(4e)	O II
$\mathbf{B}_{15}$	$= x_6 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$ax_6 \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}}$	(4f)	H II
$\mathbf{B}_{16}$	$= -(x_6 - \frac{1}{2}) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$-a(x_6 - \frac{1}{2}) \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}}$	(4f)	H II
$\mathbf{B}_{17}$	$= -x_6 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_6 \mathbf{a}_3$	$=$	$-ax_6 \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} - cz_6 \hat{\mathbf{z}}$	(4f)	H II
$\mathbf{B}_{18}$	$= (x_6 + \frac{1}{2}) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_6 \mathbf{a}_3$	$=$	$a(x_6 + \frac{1}{2}) \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} - cz_6 \hat{\mathbf{z}}$	(4f)	H II

References

- [1] C. S. Choi, J. E. Mapes, and E. Prince, *The structure of ammonium nitrate (IV)*, Acta Crystallogr. Sect. B **28**, 1357–1361 (1972), doi:10.1107/S0567740872004303.
- [2] C. D. West, *The Crystal Structure of Rhombic Ammonium Nitrate*, J. Am. Chem. Soc. **54**, 2256–2260 (1932), doi:10.1021/ja01345a013.
- [3] C. Hermann, O. Lohrmann, and H. Philipp, eds., *Strukturbericht Band II 1928-1932* (Akademische Verlagsgesellschaft M. B. H., Leipzig, 1937).

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.