

NH₄NO₃ III (*G*0₁₀) Structure: ABC3_oP20_62_c_c_cd-002

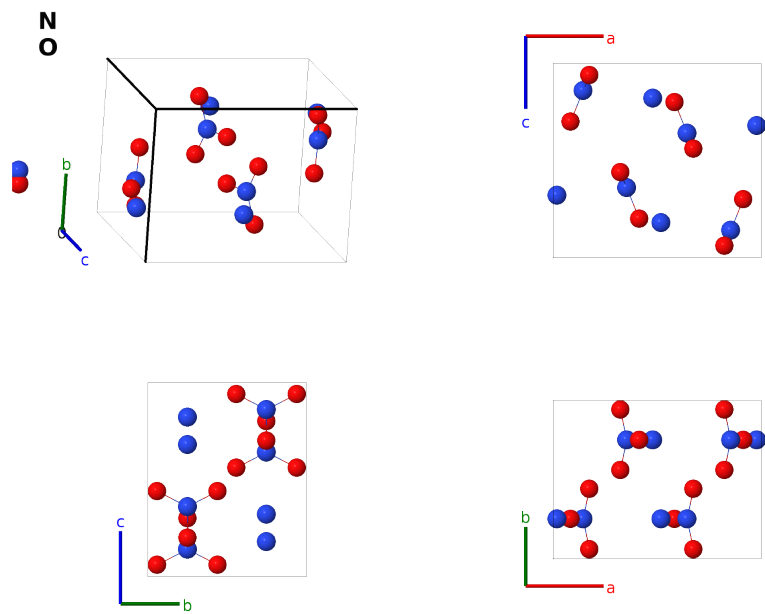
This structure previously used the label(s) `ABC3_oP20_62_c_c_cd.N.NH4.O`. Calls to these addresses will be redirected here.

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<https://aflow.org/prototype-encyclopedia/8RDG>

https://aflow.org/prototype-encyclopedia/ABC3_oP20_62_c_c_cd-002



Prototype	N(NH ₄)O ₃
AFLOW prototype label	ABC3_oP20_62_c_c_cd-002
<i>Strukturbericht</i> designation	<i>G</i> 0 ₁₀
ICSD	26665
CCDC	1602055
Pearson symbol	oP20
Space group number	62
Space group symbol	<i>Pnma</i>
AFLOW prototype command	<code>aflow --proto=ABC3_oP20_62_c_c_cd-002</code> <code>--params=<i>a, b/a, c/a, x₁, z₁, x₂, z₂, x₃, z₃, x₄, y₄, z₄</i></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 (this structure)
IV	-18 – 32	$G0_{11}$	A4B2C3_oP18_59_ef_ab_af-001
V	< –18		A4B2C3_tP72_77_8d_ab2c2d_6d2-001

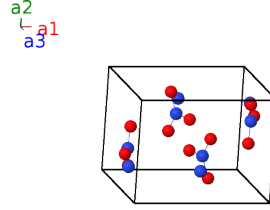
- Data for this structure was taken at 46 °C.
- It is likely that the NH_4 radicals are free to rotate (Kracek, 1937).
- (Goodwin, 1947) give the structure in the $Pbnm$ setting of space group #62. We used FINDSYM to change this to the standard $Pnma$ setting.
- Argonite (CaCO_3 , $G0_2$), $\alpha\text{-KNO}_3$, and $(\text{NH}_4)\text{NO}_3$ III ($G0_{10}$) all share the same AFLOW label, ABC3_oP20_62_c_c_cd. The structures are generated by the same symmetry operations with different sets of parameters (`--params`) specified in their corresponding CIF files.

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
$\mathbf{B}_1$	$=$	$x_1 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_1 \mathbf{a}_3$	$=$	$ax_1 \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} + cz_1 \hat{\mathbf{z}}$	(4c)	N I
$\mathbf{B}_2$	$=$	$-\left(x_1 - \frac{1}{2}\right) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \left(z_1 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a \left(x_1 - \frac{1}{2}\right) \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} + c \left(z_1 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(4c)	N I
$\mathbf{B}_3$	$=$	$-x_1 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_1 \mathbf{a}_3$	$=$	$-ax_1 \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} - cz_1 \hat{\mathbf{z}}$	(4c)	N I
$\mathbf{B}_4$	$=$	$\left(x_1 + \frac{1}{2}\right) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 - \left(z_1 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$a \left(x_1 + \frac{1}{2}\right) \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} - c \left(z_1 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(4c)	N I
$\mathbf{B}_5$	$=$	$x_2 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$ax_2 \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$	(4c)	NH I
$\mathbf{B}_6$	$=$	$-\left(x_2 - \frac{1}{2}\right) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \left(z_2 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a \left(x_2 - \frac{1}{2}\right) \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} + c \left(z_2 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(4c)	NH I
$\mathbf{B}_7$	$=$	$-x_2 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_2 \mathbf{a}_3$	$=$	$-ax_2 \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} - cz_2 \hat{\mathbf{z}}$	(4c)	NH I
$\mathbf{B}_8$	$=$	$\left(x_2 + \frac{1}{2}\right) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 - \left(z_2 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$a \left(x_2 + \frac{1}{2}\right) \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} - c \left(z_2 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(4c)	NH I
$\mathbf{B}_9$	$=$	$x_3 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$ax_3 \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(4c)	O I
$\mathbf{B}_{10}$	$=$	$-\left(x_3 - \frac{1}{2}\right) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \left(z_3 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a \left(x_3 - \frac{1}{2}\right) \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} + c \left(z_3 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(4c)	O I
$\mathbf{B}_{11}$	$=$	$-x_3 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$-ax_3 \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} - cz_3 \hat{\mathbf{z}}$	(4c)	O I
$\mathbf{B}_{12}$	$=$	$\left(x_3 + \frac{1}{2}\right) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 - \left(z_3 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$a \left(x_3 + \frac{1}{2}\right) \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} - c \left(z_3 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(4c)	O I
$\mathbf{B}_{13}$	$=$	$x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$ax_4 \hat{\mathbf{x}} + by_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(8d)	O II

$$\begin{aligned}
\mathbf{B}_{14} &= \begin{matrix} -\left(x_4 - \frac{1}{2}\right) \mathbf{a}_1 - y_4 \mathbf{a}_2 + \\ \left(z_4 + \frac{1}{2}\right) \mathbf{a}_3 \end{matrix} = -a \left(x_4 - \frac{1}{2}\right) \hat{\mathbf{x}} - by_4 \hat{\mathbf{y}} + c \left(z_4 + \frac{1}{2}\right) \hat{\mathbf{z}} & (8d) & \text{O II} \\
\mathbf{B}_{15} &= -x_4 \mathbf{a}_1 + \left(y_4 + \frac{1}{2}\right) \mathbf{a}_2 - z_4 \mathbf{a}_3 = -ax_4 \hat{\mathbf{x}} + b \left(y_4 + \frac{1}{2}\right) \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}} & (8d) & \text{O II} \\
\mathbf{B}_{16} &= \begin{matrix} \left(x_4 + \frac{1}{2}\right) \mathbf{a}_1 - \left(y_4 - \frac{1}{2}\right) \mathbf{a}_2 - \\ \left(z_4 - \frac{1}{2}\right) \mathbf{a}_3 \end{matrix} = a \left(x_4 + \frac{1}{2}\right) \hat{\mathbf{x}} - b \left(y_4 - \frac{1}{2}\right) \hat{\mathbf{y}} - c \left(z_4 - \frac{1}{2}\right) \hat{\mathbf{z}} & (8d) & \text{O II} \\
\mathbf{B}_{17} &= -x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 - z_4 \mathbf{a}_3 = -ax_4 \hat{\mathbf{x}} - by_4 \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}} & (8d) & \text{O II} \\
\mathbf{B}_{18} &= \begin{matrix} \left(x_4 + \frac{1}{2}\right) \mathbf{a}_1 + y_4 \mathbf{a}_2 - \left(z_4 - \frac{1}{2}\right) \mathbf{a}_3 \end{matrix} = a \left(x_4 + \frac{1}{2}\right) \hat{\mathbf{x}} + by_4 \hat{\mathbf{y}} - c \left(z_4 - \frac{1}{2}\right) \hat{\mathbf{z}} & (8d) & \text{O II} \\
\mathbf{B}_{19} &= x_4 \mathbf{a}_1 - \left(y_4 - \frac{1}{2}\right) \mathbf{a}_2 + z_4 \mathbf{a}_3 = ax_4 \hat{\mathbf{x}} - b \left(y_4 - \frac{1}{2}\right) \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}} & (8d) & \text{O II} \\
\mathbf{B}_{20} &= \begin{matrix} -\left(x_4 - \frac{1}{2}\right) \mathbf{a}_1 + \left(y_4 + \frac{1}{2}\right) \mathbf{a}_2 + \\ \left(z_4 + \frac{1}{2}\right) \mathbf{a}_3 \end{matrix} = -a \left(x_4 - \frac{1}{2}\right) \hat{\mathbf{x}} + b \left(y_4 + \frac{1}{2}\right) \hat{\mathbf{y}} + c \left(z_4 + \frac{1}{2}\right) \hat{\mathbf{z}} & (8d) & \text{O II}
\end{aligned}$$

References

- [1] T. H. Goodwin and J. Whetstone, *The crystal structure of ammonium nitrate III, and atomic scattering factors in ionic crystals*, J. Chem. Soc. **0**, 1455–1461 (1947), doi:10.1039/JR9470001455.
- [2] C. Hermann, O. Lohrmann, and H. Philipp, eds., *Strukturbericht Band II 1928-1932* (Akademische Verlagsgesellschaft M. B. H., Leipzig, 1937).
- [3] F. C. Kracek, S. B. Hendricks, and E. Posnjak, *Group Rotation in Solid Ammonium and Calcium Nitrates*, Nature **128**, 410–411 (1931), doi:10.1038/128410b0.

Found in

- [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.

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