# NH$_4$NO$_3$ III ($G0_{10}$) Structure: ABC3_oP20_62_c_c_cd-002
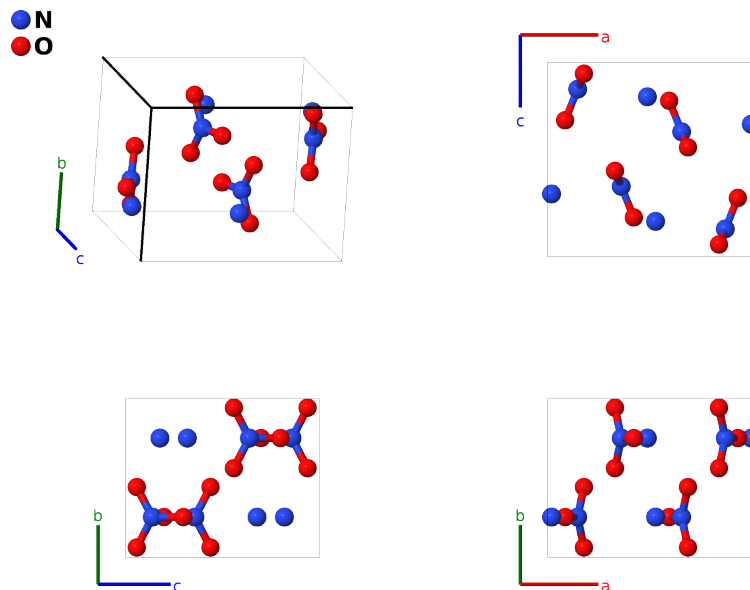
This structure originally had the label `ABC3_oP20_62_c_c_cd.N.NH4.O`. Calls to that address will be redirected here.

https://aflow.org/p/8RDG

https://aflow.org/p/ABC3_oP20_62_c_c_cd-002



| Prototype | N(NH$_4$)O$_3$ |
|---|---|
| **AFLOW prototype label** | ABC3_oP20_62_c_c_cd-002 |
| ***Strukturbericht* designation** | $G0_{10}$ |
| **ICSD** | 26665 |
| **Pearson symbol** | oP20 |
| **Space group number** | 62 |
| **Space group symbol** | $Pnma$ |
| **AFLOW prototype command** | aflow --proto=ABC3_oP20_62_c_c_cd-002 <br> --params=$a, b/a, c/a, x_1, z_1, x_2, z_2, x_3, z_3, x_4, y_4, z_4$ |

- 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 |
| 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 $46\,^{\circ}\mathrm{C}$.

- 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 ($CaCo_3$, $G0_2$), $\alpha$-$KNO_3$, and $(NH_4)NO_3$ 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.

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## Simple Orthorhombic primitive vectors

$$\mathbf{a_1} = a\,\hat{\mathbf{x}}$$
$$\mathbf{a_2} = b\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$



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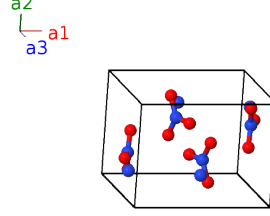
## Basis vectors

| | | 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 |
| $\mathbf{B_{14}}$ | $=$ | $-\left(x_4 - \frac{1}{2}\right)\mathbf{a_1} - y_4\,\mathbf{a_2} + \left(z_4 + \frac{1}{2}\right)\mathbf{a_3}$ | $=$ | $-a\left(x_4 - \frac{1}{2}\right)\hat{\mathbf{x}} - by_4\,\hat{\mathbf{y}} + c\left(z_4 + \frac{1}{2}\right)\hat{\mathbf{z}}$ | (8d) | 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) | O II |
| $\mathbf{B_{16}}$ | $=$ | $\left(x_4 + \frac{1}{2}\right)\mathbf{a_1} - \left(y_4 - \frac{1}{2}\right)\mathbf{a_2} - \left(z_4 - \frac{1}{2}\right)\mathbf{a_3}$ | $=$ | $a\left(x_4 + \frac{1}{2}\right)\hat{\mathbf{x}} - b\left(y_4 - \frac{1}{2}\right)\hat{\mathbf{y}} - c\left(z_4 - \frac{1}{2}\right)\hat{\mathbf{z}}$ | (8d) | 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) | O II |
| $\mathbf{B_{18}}$ | $=$ | $\left(x_4 + \frac{1}{2}\right)\mathbf{a_1} + y_4\,\mathbf{a_2} - \left(z_4 - \frac{1}{2}\right)\mathbf{a_3}$ | $=$ | $a\left(x_4 + \frac{1}{2}\right)\hat{\mathbf{x}} + by_4\,\hat{\mathbf{y}} - c\left(z_4 - \frac{1}{2}\right)\hat{\mathbf{z}}$ | (8d) | O II |

$$\mathbf{B_{19}} = x_4\,\mathbf{a}_1 - \left(y_4 - \tfrac{1}{2}\right)\mathbf{a}_2 + z_4\,\mathbf{a}_3 = ax_4\,\hat{\mathbf{x}} - b\left(y_4 - \tfrac{1}{2}\right)\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}} \quad \text{(8d)} \qquad \text{O II}$$

$$\mathbf{B_{20}} = -\left(x_4 - \tfrac{1}{2}\right)\mathbf{a}_1 + \left(y_4 + \tfrac{1}{2}\right)\mathbf{a}_2 + \left(z_4 + \tfrac{1}{2}\right)\mathbf{a}_3 = -a\left(x_4 - \tfrac{1}{2}\right)\hat{\mathbf{x}} + b\left(y_4 + \tfrac{1}{2}\right)\hat{\mathbf{y}} + c\left(z_4 + \tfrac{1}{2}\right)\hat{\mathbf{z}} \quad \text{(8d)} \qquad \text{O II}$$

## 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 Soid Ammonium and Calcium Nitrates*, Nature **128**, 410–411 (1931), doi:10.1038/128410b0.

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[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.