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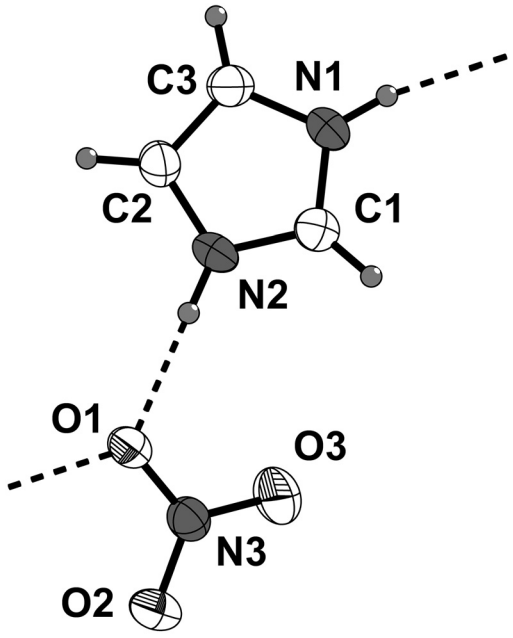
# The crystal structure of imidazolium nitrate, $C_3H_5O_3N_3$

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**Abstract**

$C_3H_5O_3N_3$, tetragonal, $P4_32_12$ (no. 96), $a$ = 7.2479(2) Å, $c$ = 21.6138(8) Å, $V$ = 1135.42(8) Å$^3$, $Z$ = 8, $R_{gt}(F)$ = 0.0344, $wR_{ref}(F^2)$ = 0.0903, T = 100 K.

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The molecular structure is shown in the figure. Table 1 contains crystallographic data and Table 2 contains the list of the atoms including atomic coordinates and displacement parameters.

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**Table 1:** Data collection and handling.

| | |
|---|---|
| Crystal: | Colourless block |
| Size: | 0.24 × 0.22 × 0.22 mm |
| Wavelength: | Cu $K\alpha$ radiation (1.54184 Å) |
| $\mu$: | 1.20 mm$^{-1}$ |
| Diffractometer, scan mode: | XtaLAB AFC12 (RINC), $\omega$ |
| $\theta_{max}$, completeness: | 75.0°, >99% |
| $N(hkl)_{measured}$, $N(hkl)_{unique}$, $R_{int}$: | 4333, 1151, 0.030 |
| Criterion for $I_{obs}$, $N(hkl)_{gt}$: | $I_{obs} > 2\sigma(I_{obs})$, 1113 |
| $N(param)_{refined}$: | 82 |
| Programs: | Olex2 [1], Shelx [2, 3], Bruker [4] |

## Source of material

An amount of 18.5 g of 15% nitric acid was added to the reactor. Weigh 3 g of imidazole for standby. Keep the temperature below 283 K, add a small amount of imidazole to 15% nitric acid for many times. After all imidazole was added, the reaction continued for 30 min. After the reaction, pour the reaction solution into the evaporating dish. Evaporate at room temperature to obtain white solid. Weigh 3 g of the above solid and dissolve it in 5 mL of water. Filter the solution to obtain a clear filtrate. At room temperature, the filtrate evaporated to obtain colorless block crystals and X-ray single crystal diffraction was performed on one of these crystals.

## Experimental details

Hydrogen atoms were placed in their geometrically idealized positions and constrained to ride on their parent atoms. All the non-hydrogen atoms were refined anisotropically.

## Comment

Energetic ionic salts have become the focus of research in the field of energetic materials in recent years [5–8]. Among them, imidazole as a skeleton is widely used in the design of energetic ionic salts [9, 10]. In this report we describe the reaction of imidazole with 15% nitric acid to obtain the title compound.

The asymmetric unit of the title compound includes a imidazole cation and a nitrate anion. The bond lengths and

**Table 2:** Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å$^2$).

| Atom | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| O1 | 0.5792 (2) | 1.07099 (19) | 0.42189 (6) | 0.0359 (4) |
| O2 | 0.5847 (3) | 1.2282 (2) | 0.50667 (7) | 0.0516 (5) |
| O3 | 0.5860 (4) | 0.9331 (2) | 0.50992 (9) | 0.0686 (6) |
| N3 | 0.5838 (2) | 1.0775 (2) | 0.48062 (8) | 0.0333 (4) |
| N1 | 0.5053 (2) | 0.4230 (2) | 0.37777 (8) | 0.0312 (4) |
| H1 | 0.526462 | 0.309005 | 0.386224 | 0.037* |
| N2 | 0.5113 (2) | 0.7183 (2) | 0.38210 (8) | 0.0312 (4) |
| H2 | 0.536802 | 0.828866 | 0.393786 | 0.037* |
| C1 | 0.5710 (3) | 0.5658 (3) | 0.40883 (9) | 0.0318 (4) |
| H1A | 0.646354 | 0.559803 | 0.443590 | 0.038* |
| C2 | 0.4021 (3) | 0.6720 (3) | 0.33267 (9) | 0.0359 (5) |
| H2A | 0.342199 | 0.753258 | 0.306117 | 0.043* |
| C3 | 0.3981 (3) | 0.4860 (3) | 0.32989 (9) | 0.0360 (5) |
| H3 | 0.334967 | 0.414399 | 0.301123 | 0.043* |

angles within these moieties are in the expected ranges [8]. Both ions are almost flat and the dihedral angle between their planes is 35.1°. N–H···O hydrogen bonds connect the cations and anions to chains along the b-axis (see the figure) and the dihedral angle is 35.120°.

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**Conflict of interest statement:** The authors declare no conflicts of interest regarding this article.

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