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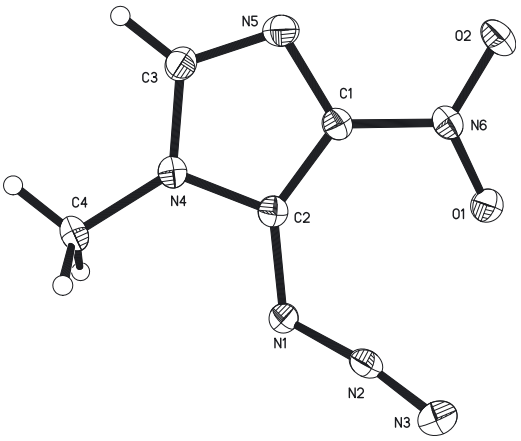
# The crystal structure of 5-azido-1-methyl-4-nitroimidazole, $C_4H_4O_2N_6$

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**Abstract**

$C_4H_4O_2N_6$, monoclinic, $P2_1/c$ (no. 14), $a$ = 11.633(3) Å, $b$ = 8.899(3) Å, $c$ = 6.7638(18) Å, $\beta$ = 105.216(12)°, $V$ = 675.6(4) Å$^3$, $Z$ = 4, $R_{gt}(F)$ = 0.0607, $wR_{ref}(F^2)$ = 0.1617, T = 170 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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## Source of material

An amount of 0.2 g of 5-azido-1-methyl-4-nitroimidazole was added to 5 ml of acetone and evaporated at room temperature to give colorless block crystals.

## Experimental details

Hydrogen atom was placed in their geometrically idealized positions and constrained to ride on their parent atoms.

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

| | |
|---|---|
| Crystal: | Colourless plate |
| Size: | 0.11 × 0.08 × 0.02 mm |
| Wavelength: | Mo $K\alpha$ radiation (0.71073 Å) |
| $\mu$: | 0.14 mm$^{-1}$ |
| Diffractometer, scan mode: | D8 VENTURE, $\varphi$ and $\omega$ |
| $\theta_{max}$, completeness: | 26.3°, 99% |
| $N(hkl)_{measured}$, $N(hkl)_{unique}$, $R_{int}$: | 4814, 1354, 0.055 |
| Criterion for $I_{obs}$, $N(hkl)_{gt}$: | $I_{obs} > 2\ \sigma(I_{obs})$, 914 |
| $N(param)_{refined}$: | 110 |
| Programs: | Bruker [1], Olex2 [2], Shelx [3, 4] |

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

| Atom | $x$ | $y$ | $z$ | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| O1 | 0.3606 (2) | 0.9455 (3) | 0.2047 (4) | 0.0388 (7) |
| O2 | 0.2018 (2) | 1.0539 (3) | 0.2491 (4) | 0.0434 (7) |
| N6 | 0.2597 (2) | 0.9410 (3) | 0.2336 (4) | 0.0315 (7) |
| N4 | 0.1775 (2) | 0.5581 (3) | 0.2405 (4) | 0.0300 (7) |
| N5 | 0.0929 (2) | 0.7820 (3) | 0.2476 (4) | 0.0326 (7) |
| N2 | 0.4627 (3) | 0.6857 (3) | 0.3347 (5) | 0.0349 (7) |
| N1 | 0.3759 (2) | 0.6082 (3) | 0.2364 (5) | 0.0339 (7) |
| N3 | 0.5485 (3) | 0.7402 (4) | 0.4153 (6) | 0.0485 (9) |
| C1 | 0.2093 (3) | 0.7975 (3) | 0.2460 (5) | 0.0281 (7) |
| C2 | 0.2643 (3) | 0.6616 (4) | 0.2429 (5) | 0.0279 (7) |
| C3 | 0.0771 (3) | 0.6361 (4) | 0.2425 (5) | 0.0319 (8) |
| H3 | 0.003321 | 0.589586 | 0.240346 | 0.038* |
| C4 | 0.1907 (3) | 0.3942 (4) | 0.2392 (6) | 0.0358 (8) |
| H4A | 0.220754 | 0.364519 | 0.122484 | 0.054* |
| H4B | 0.113169 | 0.346771 | 0.227407 | 0.054* |
| H4C | 0.247008 | 0.361950 | 0.366867 | 0.054* |

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## Comment

The imidazole ring has high reactivity when C-5 is azide group or chlorine, and which can be used to prepare biologically active compounds [5–9]. 5–Azido- 1-methyl-4-nitroimidazole is one of their representatives?? which reacted with endocyclic enamines [6], alicyclic amines [7], cyclic ketones [7], triphenylphosphine [8] or triethyl phosphite [9] to give compounds with high biological activity. In this paper, the title compound was obtained by azide reaction of 4,5-MDNI with sodium azide [10].

The crystal structure of the title compound was analyzed and refined using the SHELLX program [1–4]. As shown in the figure, the asymmetric unit of the title compound contains one title molecule. The bond lengths and angles within these moieties are in the expected ranges. The imidazole rings are planar, the carbon atoms of the methyl group and the nitro group are nearly coplanar with the imidazole ring. However, the hydrogen atoms of the methyl group and the azido group are twist out of the imidazole ring.

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