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Crystal structure of 1*H*-1,2,3-Triazolo[4,5-*b*]-pyridin-4-ium nitrate, C₅H₅N₅O₃

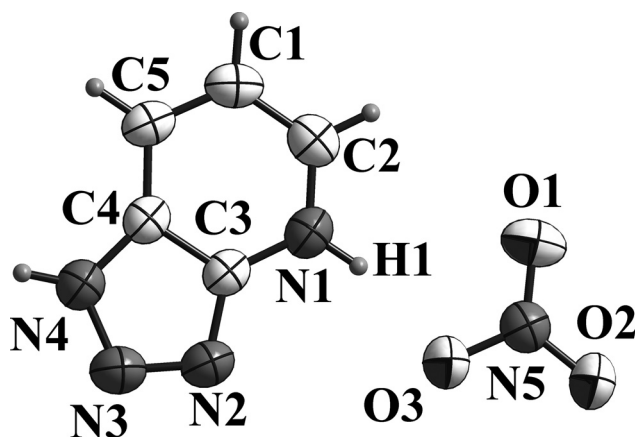


Table 1: Data collection and handling.

Crystal:	Colourless plate
Size:	0.40 × 0.30 × 0.20 mm
Wavelength:	Mo K α radiation (0.71073 Å)
μ :	0.13 mm ⁻¹
Diffractometer, scan mode:	SuperNova, ω
$\theta_{\max}$, completeness:	28.9°, >99%
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$, R_{int} :	2217, 1108, 0.012
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 741
$N(\text{param})_{\text{refined}}$:	79
Programs:	CrysAlis ^{PRO} [1], Olex2 [2], SHELX [3, 4]

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Abstract

C₅H₅N₅O₃, orthorhombic, *Pnma* (no. 62), $a = 13.4643(13)$ Å, $b = 6.2866(10)$ Å, $c = 9.1138(9)$ Å, $V = 771.43(16)$ Å³, $Z = 4$, $R_{\text{gt}}(F) = 0.0517$, $wR_{\text{ref}}(F^2) = 0.1317$, $T = 293$ K.

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Table 1 contains crystallographic data and Table 2 contains the list of the atoms including atomic coordinates and displacement parameters.

Source of material

In a typical experiment, a mixture of 1*H*-1,2,3-triazolo[4,5-*b*]pyridine, (0.3 mmol, 36 mg), HNO₃, (65%, 0.2 mL), and water 10 mL was placed in a glass vessel, kept at ambient conditions for 15 days. Colourless block crystals of the title compound were obtained.

Table 2: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²).

Atom	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	0.95226 (19)	0.2500	0.5360 (3)	0.0551 (7)
H1A	1.0061	0.2500	0.4721	0.066*
C2	0.8569 (2)	0.2500	0.4794 (3)	0.0579 (7)
H2	0.8478	0.2500	0.3782	0.070*
C3	0.79131 (16)	0.2500	0.7123 (3)	0.0466 (6)
C4	0.88521 (16)	0.2500	0.7715 (3)	0.0448 (6)
C5	0.96904 (18)	0.2500	0.6839 (3)	0.0512 (6)
H5	1.0328	0.2500	0.7232	0.061*
N1	0.77829 (15)	0.2500	0.5670 (2)	0.0548 (6)
H1	0.7194	0.2500	0.5306	0.066*
N2	0.72187 (15)	0.2500	0.8185 (2)	0.0622 (7)
N3	0.76899 (17)	0.2500	0.9432 (3)	0.0664 (7)
N4	0.86665 (16)	0.2500	0.9174 (2)	0.0563 (6)
H4	0.9116	0.2500	0.9844	0.068*
N5	0.56712 (16)	0.2500	0.3625 (2)	0.0532 (6)
O1	0.63642 (15)	0.2500	0.2767 (2)	0.0709 (6)
O2	0.47945 (14)	0.2500	0.3212 (2)	0.0756 (7)
O3	0.58244 (13)	0.2500	0.49944 (19)	0.0715 (7)

Experimental details

Using Olex2 [2], the structure was solved with the ShelXT [3] structure solution program using Intrinsic Phasing and refined with the ShelXL [4] refinement package. Hydrogen atom was placed in their geometrically idealized positions and constrained to ride on their parent atoms.

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Comment

1*H*-1,2,3-Triazolo[4,5-*b*]pyridine molecule was widely used in synthetic chemistry [5, 6], optical chemistry [7, 8], and medical chemistry [9, 10]. Commonly, it was used in aqueous solution, in order to increase the solubility. We investigated the stability of this compound in alkaline and acidic solutions. Besides, the approach of crystal engineering can provide the most straightforward and visual structure information [11–14]. To the best of our knowledge the title compound is reported for the first time.

The single-crystal X-ray diffraction analysis revealed that synthesized compound crystallize in the orthorhombic system with a *Pnma* space group. The asymmetric unit of the title compound includes a cation and a nitrate anion (see the Figure). The bond lengths and angles within these moieties are in the expected ranges [15]. Five carbon atoms and four nitrogen atoms in the cation are in the same plane. More interestingly, the plane formed by the cation is almost the same as that formed by nitrate ions. The anions and cations are connected by hydrogen bonds.

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