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The crystal structure of 3-amino-1,2,4-triazolium 2,4,5-trinitroimidazolate, $C_5H_5O_6N_9$

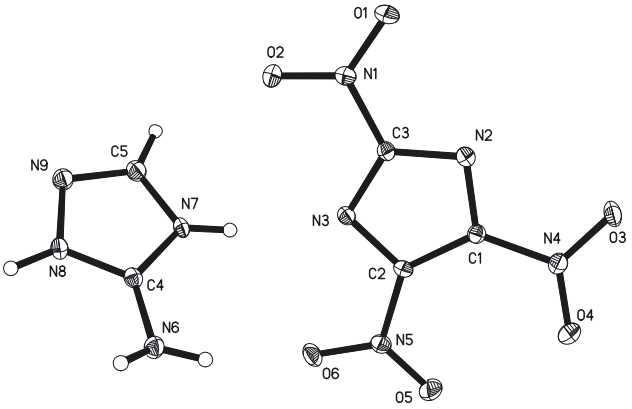

Table 1: Data collection and handling.

Crystal:	Colourless block
Size:	0.15 × 0.08 × 0.05 mm
Wavelength:	Mo *K*α radiation (0.71073 Å)
μ:	0.17 mm^{-1}
Diffractometer, scan mode:	D8 VENTURE, φ and ω
θ_{max}, completeness:	26.4°, >99%
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	11426, 2104, 0.050
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\ \sigma(I_{obs})$, 1876
$N(param)_{refined}$:	198
Programs:	Bruker [1], Olex2 [2], SHELX [3, 4]

https://doi.org/10.1515/ncrs-2022-0321
Received June 21, 2022; accepted July 15, 2022;
published online August 8, 2022

Abstract

$C_5H_5O_6N_9$, orthorhombic, $P2_12_12_1$ (no. 19), a = 5.6068(2) Å, b = 10.0191(4) Å, c = 18.3799(8) Å, V = 1032.49(7) Å^3, Z = 4, $R_{gt}(F)$ = 0.0340, $wR_{ref}(F^2)$ = 0.0776, T = 140 K, β = 90.

CCDC no.: 2044766

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.

Source of material

0.2 g of 3-amino-1,2,4-triazolium 2,4,5-trinitroimidazolate was added to 10 ml of methanol and evaporated at room temperature to give colorless block crystals. X-ray single crystal diffraction was performed on the crystal.

Experimental details

The H5 atom was placed in its geometrically idealized position and constrained to ride on the C5 parent atom with U_{iso} = 1.2U_{eq}. The positions of hydrogen atoms at the nitrogen atoms were determined from electron density difference maps and refined using isotropic approximation. All the non-hydrogen atoms were refined anisotropically.

Comment

Nitroimidazole compounds are an important class of energetic materials [5–15], and ionic salt of 2,4,5-trinitroimidazole is one of their representatives. 3-Amino-1,2,4-triazolium 2,4,5-trinitroimidazolate was first synthesized by Gao et al. However, the starting materials were easily introduced into the product following the synthetic procedures of the Gao's literature [11]. In this paper, the title compound was synthesized by adding dropwise a solution of 3-amino-1,2,4-triazole in ethanol to a solution of 2,4,5-trinitroimidazole in ether, which was obtained in precipitated form [14].

The crystal structure of the title compound was analyzed and refined by ShelXL program [3, 4]. As shown in the figure, the asymmetric unit of the title compound contains the

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

Atom	*x*	*y*	*z*	U_{iso}*/U_{eq}
O1	0.1581 (4)	0.3467 (2)	0.40202 (11)	0.0289 (5)
O2	0.1356 (4)	0.33102 (19)	0.51979 (11)	0.0236 (5)
O3	0.8714 (4)	0.6139 (2)	0.32868 (10)	0.0260 (5)
O4	1.0630 (5)	0.6970 (2)	0.41970 (12)	0.0440 (7)
O5	1.0795 (4)	0.6398 (2)	0.56244 (11)	0.0327 (5)
O6	0.8268 (4)	0.5552 (2)	0.63872 (10)	0.0277 (5)
N1	0.2340 (4)	0.3684 (2)	0.46367 (13)	0.0189 (5)
N2	0.5578 (4)	0.4958 (2)	0.41201 (12)	0.0172 (5)
N3	0.5467 (4)	0.4683 (2)	0.53523 (12)	0.0169 (5)
N4	0.9062 (4)	0.6282 (2)	0.39414 (13)	0.0206 (5)
N5	0.8926 (4)	0.5829 (2)	0.57685 (12)	0.0199 (5)
C1	0.7446 (5)	0.5586 (3)	0.44219 (14)	0.0167 (6)
C2	0.7374 (5)	0.5419 (3)	0.51797 (14)	0.0165 (6)
C3	0.4495 (5)	0.4454 (3)	0.47035 (14)	0.0162 (6)
N6	0.3564 (5)	0.6117 (2)	0.72791 (14)	0.0221 (6)
H6A	0.250 (6)	0.668 (3)	0.7452 (18)	0.036 (10)*
H6B	0.469 (5)	0.633 (3)	0.6983 (16)	0.038 (10)*
N7	0.3411 (5)	0.3964 (2)	0.67237 (13)	0.0198 (5)
H7	0.433 (6)	0.410 (3)	0.6372 (17)	0.026 (9)*
N8	0.1117 (4)	0.4287 (2)	0.76341 (13)	0.0192 (5)
H8	0.037 (7)	0.458 (3)	0.8021 (18)	0.035 (10)*
N9	0.0681 (5)	0.2991 (2)	0.74079 (13)	0.0235 (6)
C4	0.2739 (5)	0.4878 (3)	0.72159 (14)	0.0175 (6)
C5	0.2107 (6)	0.2843 (3)	0.68597 (16)	0.0234 (6)
H5	0.223127	0.204449	0.658366	0.028*

2,4,5-trinitroimidazole anion and the 3-amino-1,2,4-triazole cation. The bond lengths and angles within these moieties are in the expected ranges. The imidazole ring and 1,2,4-triazole ring are planar. The oxygen atoms of nitro groups and the hydrogen atoms of amino group are twisted out the imidazole ring and 1,2,4-triazole ring, respectively.

Author contributions: All the authors have accepted responsibility for the entire content of this submitted manuscript and approved submission.

Research funding: This work is supported by the Scientific and Technological Innovation Programs of Higher Education Institutions in Shanxi (Grant No. 2019L0606), and the Fundamental Research Program of Shanxi Province (Grant No. 202103021223201).

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

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