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Short Note

(*E*)-1-(5-Methyl-1-(4-nitrophenyl)-1*H*-1,2,3-triazol-4-yl)ethan-1-one Oxime

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Abstract: The reaction of 1-(5-methyl-1-(4-nitrophenyl)-1*H*-1,2,3-triazol-4-yl)ethan-1-one (**1**) with excess hydroxylamine hydrochloride (2 mole equivalents) in dry ethanol afforded (*E*)-1-(5-methyl-1-(4-nitrophenyl)-1*H*-1,2,3-triazol-4-yl)ethan-1-one oxime (**2**) in 86% yield. The structure of the new heterocycle **2** was confirmed using nuclear magnetic resonance spectroscopy, single crystal X-ray and elemental analysis.

Keywords: triazoles; oximes; hydroxylamine hydrochloride; X-ray diffraction; heterocycles; synthesis

Citation: Abdel-Wahab, B.F.; Farahat, A.A.; Kariuki, B.M.; El-Hiti, G.A. (*E*)-1-(5-Methyl-1-(4-nitrophenyl)-1*H*-1,2,3-triazol-4-yl)ethan-1-one Oxime. *Molbank* **2023**, *2023*, M1593. https://doi.org/10.3390/M1593

Academic Editor: Fawaz Aldabbagh

Received: 15 January 2023
Revised: 14 February 2023
Accepted: 19 February 2023
Published: 21 February 2023

1. Introduction

Oximes are a class of imines with the general formula R^1R^2C=N–OH. They are primarily obtained from condensing hydroxylamine and carbonyl compounds (aldehydes or ketones). Aldoximes are produced from aldehyde, whereas ketoximes are synthesized from ketones [1–3]. Oximes have unique properties and act as nucleophiles due to the presence of nitrogen and oxygen atoms. In addition, oximes contain an ambiphilic carbon and are considered strong candidates for divergent reactivity [4].

For many years, oximes have been investigated due to their significant potential as acetylcholinesterase reactivators and in the cure for several diseases [5–8]. Oximes with different scaffolds have shown activity against bacterial infections, including tuberculosis [9]. In addition, oximes act as anti-inflammatory reagents [10–12], and their activity is comparable to standard drugs such as indomethacin, dexamethasone, and diclofenac [13]. Moreover, oximes are an active component of various kinase inhibitors such as phosphatidyl inositol 3-kinase [14], phosphorylase kinase [15], and c-Jun N-terminal kinase [16].

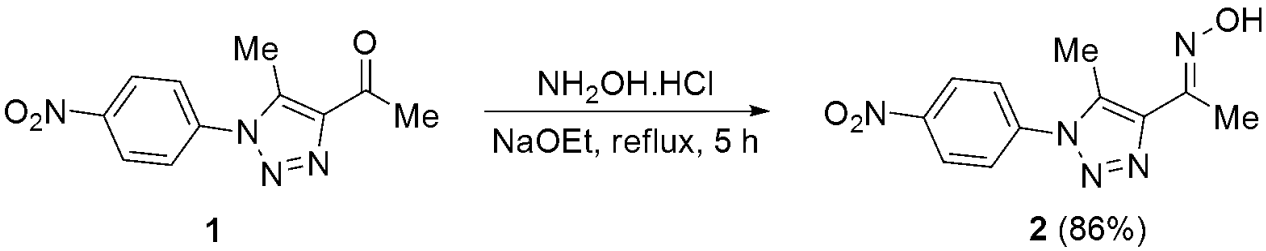
Heterocycles containing 1,2,3-triazole moiety have various biological activities [17–22]. For example, several novel 1,2,3-triazoles have been synthesized and their anticancer activity was investigated. Some of the synthesized 1,2,3-triazoles showed potential as anticancer (e.g., lung cancer) drugs [23,24]. The most common synthetic method used to produce 1,2,3-triazole ring systems involves click chemistry [25]. The synthetic processes that employ click chemistry are simple, efficient, and produce a range of substituted 1,2,3-triazoles in good yields [26]. In addition, 1,2,3-triazoles can be synthesized efficiently from the 1,3-cycloaddition of active methylene compounds containing nitriles and aryl azides [27]. 1,2,3-Triazolyl-based ketoximes can be synthesized from the reaction of calcium carbide (an acetylene source) and (*Z*)-2-azido-1-arylethan-1-one oximes [28]. 1,2,3-Triazole oximes can be also synthesized from the reaction of 4-acetyl-1,2,3-triazoles and hydroxylamine hydrochloride in an acidic medium [29]. The synthesis of heterocycles containing both

oxime and 1,2,3-triazole moieties is an interesting proposition. Recently, we have synthesized a range of heterocycles containing 1,2,3-triazole ring systems [30–35]. The aim of the current work was to synthesize a novel heterocycle containing both oxime and 1,2,3-triazole moieties using a facile and routine method. The synthesis of such a compound opens gates for the production of a series of derivatives containing various substituents to test their effect on the biological activities of 1,2,3-triazoles containing oxime.

2. Results and Discussion

2.1. Synthesis

The condensation of 1-(5-methyl-1-(4-nitrophenyl)-1*H*-1,2,3-triazol-4-yl)ethan-1-one (**1**) with excess hydroxylamine hydrochloride ($H_2NOH.HCl$) in dry EtOH afforded (*E*)-1-(5-methyl-1-(4-nitrophenyl)-1*H*-1,2,3-triazol-4-yl)ethan-1-one oxime (**2**) (Scheme 1). The progress of the reaction was tested using thin layer chromatography. A reflux for 5 hours was need for the reaction to be completed. Crystallization of the crude product using dimethylformamide (DMF) led to crystals of **2** in 86% yield.



Scheme 1. Synthesis of 1,2,3-triazole oxime **2**.

2.2. NMR Spectroscopy

The ^{1}H NMR spectrum of **2** showed the presence of an exchangeable singlet that appeared at 11.28 ppm due to the hydroxyl proton. In addition, it showed the presence of two methyl groups that appeared at 2.23 and 2.48 ppm. The protons of the aryl ring appeared as two doublets (J = 9.1 Hz) at 7.92 and 8.4q ppm. The ^{13}C NMR spectrum of **2** showed the C=N–OH carbon appeared at a high downfield at 154.2 ppm. The two methyl carbons appeared at 15.8 and 17.3 ppm, and C1 and C4 of the aryl ring appeared at 145.8 and 152.9 ppm, respectively. See Supplementary materials for details.

2.3. X-ray Crystal Structure

The crystal structure contained two independent molecules of **2**, M_1 and M_2 (Figure 1). Each molecule comprised nitrobenzene (M_1A: C1–C4, N1, O1, O2 and M_2A: C12–C17, N6, O4, O5), triazole (M_1B: C7–C9, N2–N4 and M_2B: C18–C20, N7–N9), and (ethylidene)hydroxylamine (M_1C: C10, C11, N5, O3 and M_2C: C23, C24, N10, O6) moieties.

The nitro group of molecule M_2 was coplanar with the benzene ring it was attached to (the twist angle was 5.9(3)°), whereas the group was disordered in M_1, with twists of approximately 15° from the plane of the corresponding benzene ring. The triazole and (ethylidene)hydroxylamine groups were coplanar in both molecules, with twist angles M_1B/M_1C and M_2B/M_2C of 4.38(15)° and 7.77(12)°, respectively. In both molecules, the benzene rings were twisted from the planes of the triazole ring with twist angles of 35.7(1)° and 47.7(1)°.

In the crystal, the molecules were stacked to form columns parallel to the a-axis (Figure 2a). Intermolecular O–H . . . N hydrogen bonding occured in the structure (Figure 2b). The triazole group of molecule M_2 accepted contacts from two neighbors with geometry O3–H3A . . . N9 = 164.5°, O3 . . . N9 = 2.878(3)Å and O6–H6A . . . N8 = 165.2°, O6 . . . N8 = 2.967(3) Å.

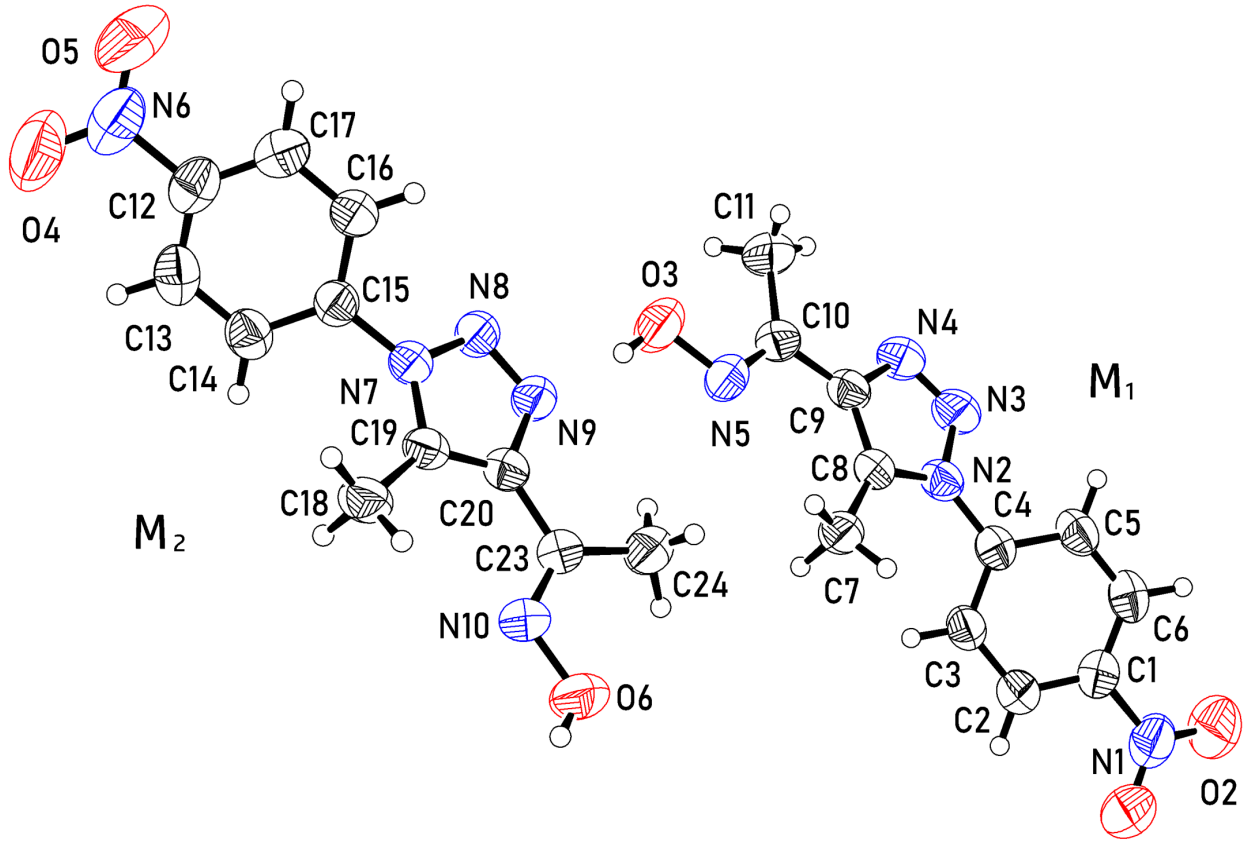
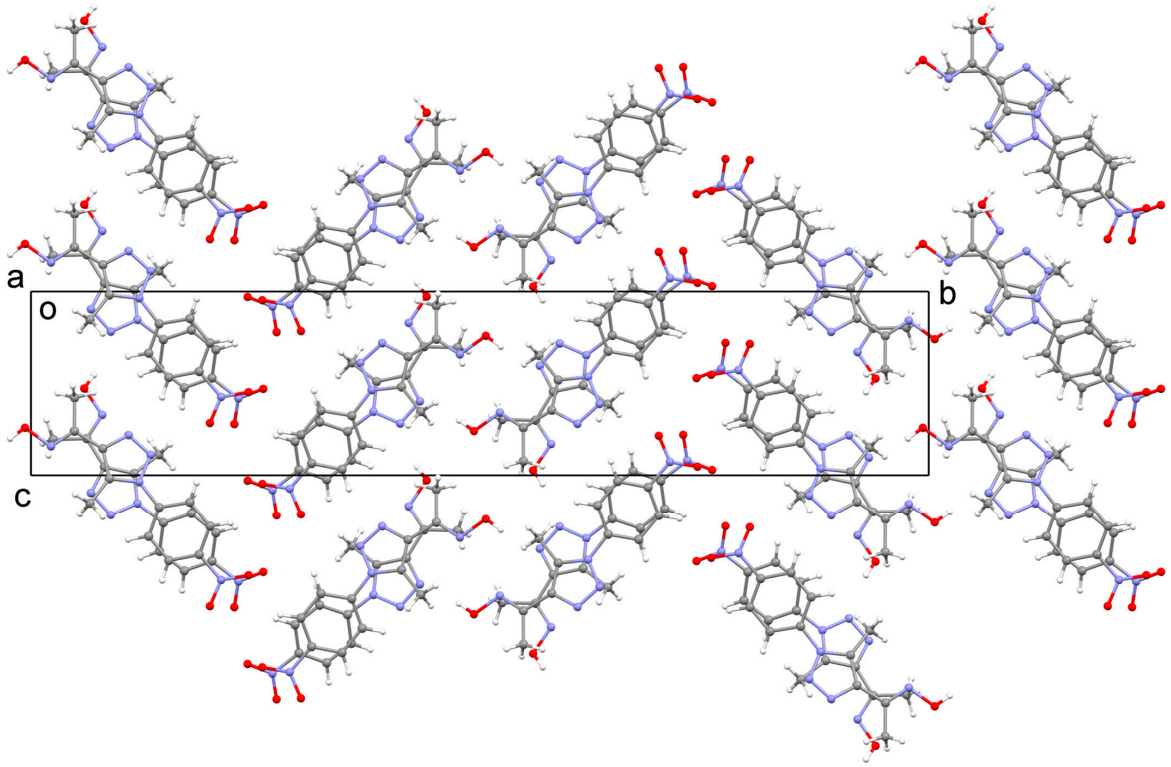
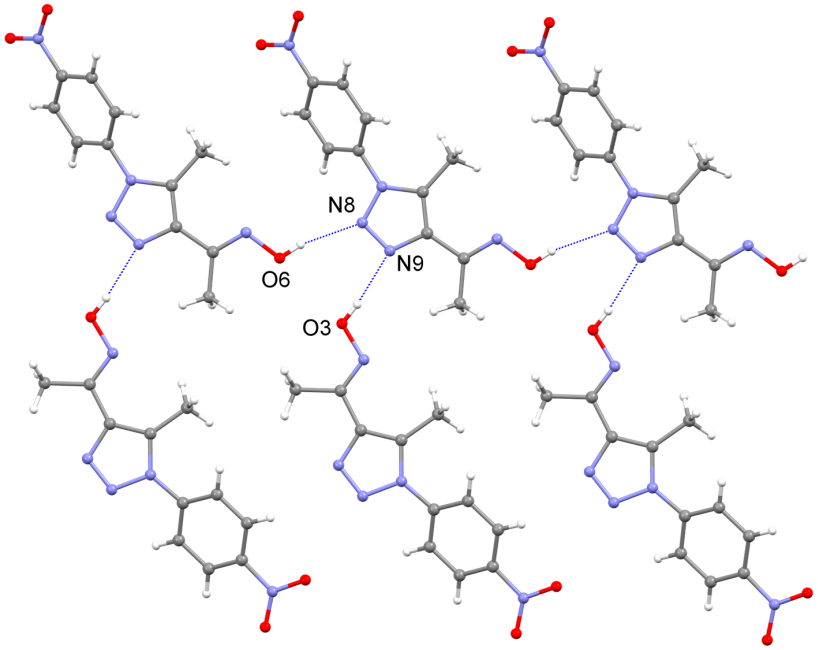


Figure 1. An ORTEP representation of the asymmetric unit of **2** showing 50% probability atomic displacement parameters.



(**a**)

Figure 2. *Cont.*



(**b**)

Figure 2. (**a**): Crystal packing and (**b**): a segment of the structure showing hydrogen bonding as blue dotted lines.

3. Materials and Methods

3.1. General

The ^{1}H (500 MHz) and ^{13}C NMR (125 MHz) spectra were assessed using a JEOLNMR spectrometer. The chemical shift (δ) was measured in ppm and, the coupling constant (*J*) was calculated in Hz. Compound **1** was produced based on a literature procedure [36].

3.2. Synthesis of 2

A mixture of methyl ketone **1** (0.63 g, 2.5 mmol) and $H_2NOH.HCl$ (0.35 g, 5.0 mmol) in dry EtOH (15 mL) was refluxed for 5 h. The mixture was left to cool to 20 °C and the solid produced was collected via filtration. The product was washed with EtOH, dried, and recrystallized from DMF to yield **2** in crystalline form in 86% yield. MP 212–213 °C. ^{1}H NMR (ppm; Hz): 2.23 (s, 3H, Me), 2.48 (s, 3H, Me), 7.92 (d, 9.1 Hz, 2H, H3/H5 of Ar), 8.41 (d, 9.1 Hz, 2H, H2/H6 of Ar), 11.28 (s, exch., 1H, OH). ^{13}C NMR (ppm): 15.8 (Me), 17.2 (Me), 130.3 (C3/C5 of Ar), 131.2 (C2/C6 of Ar), 137.2 (C4 of triazolyl), 143.4 (C5 of triazolyl), 145.8 (C1 of Ar), 152.9 (C4 of Ar), 154.2 (C=N–OH). Anal. Calcd. for $C_{11}H_{11}N_5O_3$ (261.24): C, 50.57; H, 4.24; N, 26.81. Found: C, 50.66, H, 4.54, N, 26.93%.

3.3. Crystal Structure Determination

Single-crystal XRD data were collected on an Agilent SuperNova Dual Atlas diffractometer with a mirror monochromator using Mo radiation. The crystal structure of **2** was solved and refined using SHELXT [37] and SHELXL [38]. The nitro group of one molecule was disordered with two components related by a 34.1(11)° twist about the C–N bond with occupancies of 0.52(3) and 0.48(3). Non-hydrogen atoms were refined with anisotropic displacement parameters and hydrogen atoms were inserted in idealized positions; a riding model was used with Uiso set at 1.2 or 1.5 times the value of Ueq for the atom to which they were bonded.

Molecular formula = $C_{22}H_{22}N_{10}O_6$, formula weight = 522.49, temperature = 293(2) K, wavelength = 0.71073 Å, monoclinic, $P2_1/c$, a = 7.5755(6) Å, b = 39.3294(18) Å, c = 8.3050(4) Å, α = 90°, β = 104.999(6)°, γ = 90°, volume = 2390.1(3) Å3, Z = 4, density (calculated) = 1.452 Mg/m^3, absorption coefficient = 0.110 mm^{-1}, F(000) = 1088, crystal size = 0.530 × 0.330

× 0.050 mm^3, reflections collected = 24965, independent reflections = 6011, R(int) = 0.0299, parameters = 368, goodness-of-fit on F^2 = 1.083, final R1 [I>2sigma(I)] = 0.0653, wR2 [I>2sigma(I)] = 0.1940, R1 (all data) = 0.0943, wR2 (all data) = 0.2147, largest diff. peak and hole = 0.201 and -0.250 e.$Å^{-3}$, respectively. The data have been deposited in the CSD using reference CCDC 2235605.

4. Conclusions

(*E*)-1-(5-Methyl-1-(4-nitrophenyl)-1*H*-1,2,3-triazol-4-yl)ethan-1-one oxime was synthesized in excellent yield using a simple procedure. The structure of the title heterocycle was confirmed using nuclear magnetic spectroscopy and single crystal X-ray diffraction.

Supplementary Materials: The following are available online. ^{1}H and ^{13}C NMR spectra, CIFs, and checkcif report for heterocycle **2**.

Author Contributions: Conceptualization: G.A.E.-H. and B.M.K.; methodology: B.F.A.-W., B.M.K. and G.A.E.-H.; X-ray crystal structures: B.M.K.; investigation: B.F.A.-W., A.A.F., B.M.K. and G.A.E.-H.; writing—original draft preparation: B.F.A.-W., A.A.F., B.M.K. and G.A.E.-H.; writing—review and editing: B.F.A.-W., A.A.F., B.M.K. and G.A.E.-H. All authors have read and agreed to the published version of the manuscript.

Funding: G.A.E.-H. acknowledges the support received from the Researchers Supporting Project (number RSP2023R404), King Saud University, Riyadh, Saudi Arabia.

Institutional Review Board Statement: Not applicable.

Informed Consent Statement: Not applicable.

Data Availability Statement: Data are contained within the article and the supplementary material.

Acknowledgments: We thank Cardiff University and the National Research Centre for technical support.

Conflicts of Interest: The authors declare no conflict of interest.

Sample Availability: A samples of the title compound is available from the authors.

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