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Alkylation of 3-nitro-1,2,4-triazole in the *N*-methylmorpholine *N*-oxide/water system and identifying the structure of obtained compounds

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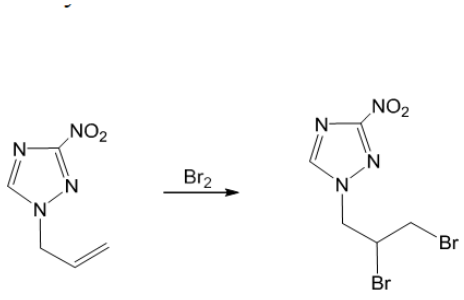
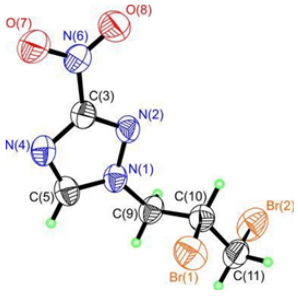
Alkylation of 3-nitro-1,2,4-triazole with alkyl halides can theoretically lead to the formation of three isomers 1-allyl-3-nitro-1,2,4-triazole (A), 2-allyl-3-nitro-1,2,4-triazole (B), and 4-allyl-3- nitro-1,2,4-triazole (C) as a result of alkylation at positions 1, 2, and 4, respectively. According to the published data, alkylation of 3-nitro-1,2,4-triazole with alkyl halides dependingon the reaction conditions proceeds with the preferred formation of the substitution product at the nitrogen atom N-1 (isomer A). However, the reaction products also contain the regioisomer B in appreciable amounts together with isomer A. In published data, unfortunately, no concrete proof of the structure of isomers A and B is given using spectral techniques. Alkylation of 3-nitro-1,2,4-triazole with allyl bromide in an aqueous alkaline medium in the presence of N-methylmorpholine-N-oxide leads to a mixture of the two isomers A and B, the predominant one corresponding to ^{1}H NMR spectrum is compound A. However, in the alkylation of triazole with allyl bromide, it is necessary to take into account the possibility of formation of the third isomer C. In this case, the NOESY experiment is not informative, since in both isomers, NOE can be observed between the protons of the methylene substituent and the methyl group of a triazole ring. In this regard, and considering that N- allyltriazoles are liquids under normal conditions, we proposed an indirect way of identifying their structures. The essence of the method is the bromination of 1-allyl-3-nitro-1,2,4-triazole in an aqueous solution of sodium acetate, which without alternative leads to the formation of 1-(2,3- dibromopropyl)-3-nitro-1,2,4 -triazole, formed in the form of crystals, which makes it possible to carry out its X-ray structural studies.





X-ray structural analysis showed that the compound obtained is a product of the addition of bromine to 1-allyl-3-nitro-1,2,4-triazole, i.e., to triazole A.

Recent Publications:

1. A.H.Hasratyan, "NMO/H_2O system as a a new medium for nucleophilic reactions", 9th GlobalChemistry Congress, July 23-24, 2018, Lisbon, Portugal, p. 31.

A.H. Hasratyan, A.G. Alexanyan, H.N. Khachatryan, G.B. Zakaryan, S.S. Hayotsyan, G.G.

Danagulyan, H.S. Attaryan, "Aqueous N-methylmorpholine N-oxide as a new medium for alky- lation of pyrazoles", Chem. of Heterocyclic Compounds, 2018, vol. 54, issue 7, pp. 751–754.

A.H. Hasratyan, G.A. Bagdasaryan, A.D. Markosyan, K.S. Badalyan, H.S. Attaryan, "Synthesis of 4-vinylmorpholine based on acetylene", Russ. J. of Applied Chem., 2018, vol. 91, issue 2, pp. 342–345.

A.H.Hasratyan, "Synthesis of 1-vinylimidazole and the study of complexation with HAuCl4", 10th European Organic Chemistry Congress, March 21-22, 2019, Rome, Italy, p. 38.

Biography

Ani Hasratyan received her master degree at Chemical faculty of Yerevan State University in 2013 under supervision of T. Ghochikyan. She received her PhD student in 2017 under supervision of Dr. M. Sargsyan. During her scientific work she has already done a lot of experiments and has 29published articles. Her research interest is NMO/H_2O system and its chemical properties in applied organic synthesis. She participated in 4th International Conference of Young Scientists "Chemistry Today-2014", August 18-22, 2014, Yerevan, Armenia, pp.122-123; IV Scientific Conference of the Armenian Chemical Society "Achievements and Problems", October 7-11, 2014, Yerevan – Vanadzor, p.158; 9th Global Chemistry Congress, July 23-24, 2018, Lisbon, Portugal, p. 31; 10th European Organic Chemistry Congress, March 21-22, 2019, Rome, Italy, p. 38 and VI Scientific Conference of the Armenian Chemical Society, October 7-11, 2019, Yerevan, Armenia, p. 20.