Determination of the 1-(2-nitrovinyl)-3-phenylpyrrolidine structure using NMR spectroscopy

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Nitroenamines attract considerable interest due to their potential in organic synthesis and biological activity [1]. The most convenient and widely used synthon in this group is N,N-dimethyl-2-nitroethen-1-amine, first synthesized as early as the 20th century [2]. However, information on the chemical properties and, particularly important, spectral data of its derivatives remain limited to this day. One of the most effective methods for obtaining diverse nitroenamines, varying by the substituent at the amino group, is the transamination reaction.

For the first time, the interaction of N,N-dimethyl-2-nitroethen-1-amine with 3-phenylpyrrolidine was carried out, leading to the formation of a new nitroenamine, which can exist as two geometric isomers, E and Z. In the ^{1}H NMR spectrum, a doubled set of signals from all structural fragments is observed, indicating the obtaining of a mixture of two substances with similar structures. The vicinal coupling constant of the olefinic protons in each of the sets are 10.5 and 10.7 Hz, which agrees with literature data for structures of related compounds existing in the E-form [1].

Thus, the reason for the doubling of signals in the ^{1}H NMR spectra is the existence of the obtained product as two conformers. This is related to the asymmetric structure of the 3-phenylpyrrolidine substituent, whose rotation around the C–N bond is hindered due to conjugation involving the lone electron pair of the nitrogen atom and the C=C bond of the nitroolefin fragment.

Therefore, based on two-dimensional NMR spectroscopy, the structure of the obtained conformers was confirmed by us.

[1] Chiara J. L., Gómez-Sánchez A., Bellanato J. J. Chem. Soc., Perkin Trans. 2. 1992. №5. P. 787-798.
[2] Severin, T., Brück, B., Adhikary, P. Ber. 1966, 99(10), 3097