Mass Spectra of New Heterocycles: XX.[1] Electron Impact and Chemical Ionization Mass Spectra of 5-(Prop-2-yn-1-ylsulfanyl)-1*H*-pyrrol-2-amines

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Received May 23, 2019; revised October 23, 2019; accepted October 24, 2019

Abstract—Electron impact (70 eV) and chemical ionization (methane as reactant gas) mass spectra of 1-alkyl- and 1-[2-(vinyloxy)ethyl]-5-(prop-2-yn-1-ylsulfanyl)-1*H*-pyrrol-2-amines have been studied for the first time. The title compounds under electron impact form stable molecular ions which decompose mainly along pathways typical of the molecular ions derived from the corresponding intramolecular cyclization products, 7-alkyl- and 7-[2-(vinyloxy)ethyl]-2,7-dihydrothiopyrano[2,3-*b*]pyrrol-6-amines. In addition, fragment ions that could be formed only via decomposition of unrearranged molecular ion were detected. The main fragmentation pathway of their molecular ions involves cleavage of the N^1–C_{Alk} bond with the formation of stable $[M - R^3]^+$ ions (I_{rel} 85–100%) {except for *N*,*N*-diethyl- and *N*,*N*-dipropyl-1-[2-(vinyloxy)ethyl]-5-(prop-2-yn-1-ylsulfanyl)-1*H*-pyrrol-2-amines}. The results of quantum chemical calculations at the B3LYP/6-311+G(*d*,*p*) level of theory are consistent with the experimental data. In the chemical ionization mass spectra of 5-(prop-2-yn-1-ylsulfanyl)-1*H*-pyrrol-2-amines, the major peaks were those corresponding to $M^{+\cdot}$ (I_{rel} 65–100%) and $[M + H]^+$ (I_{rel} 75–100%). The title compounds have been found to undergo partial (5–10%) thermally induced isomerization to 5-(prop-1-yn-1-ylsulfanyl)-1*H*-pyrrol-2-amines under the chemical ionization conditions.

Keywords: 1-alkyl- and 1-[2-(vinyloxy)ethyl]-5-(prop-2-yn-1-ylsulfanyl)-1*H*-pyrrol-2-amines, electron impact, chemical ionization, mass spectra, molecular ions, intramolecular cyclization, isomerization, fragmentation, quantum-chemical calculations.

DOI: 10.1134/S1070428019120078