Mass Spectra of New Heterocycles: X.* Fragmentation of the Molecular Ions of 1-Alkyl(cycloalkyl, aryl)-3-alkoxy(aryl)-2-methylsulfanyl-1*H*-pyrroles

L. V. Klyba, N. A. Nedolya, O. A. Tarasova, E. R. Zhanchipova, and O. G. Volostnykh

Favorskii Irkutsk Institute of Chemistry, Siberian Division, Russian Academy of Sciences,
ul. Favorskogo 1, Irkutsk, 664033 Russia
e-mail: nina@irioch.irk.ru

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Abstract—The mass spectra of previously unknown 1-alkyl(cycloalkyl, aryl)-3-alkoxy(aryl)-2-methylsulfanyl-1*H*-pyrroles were studied. Fragmentation of all 3-alkoxy-substituted pyrroles under electron impact (70 eV) follow both ether and sulfide decomposition paths; In particular, 1-R-substituted 3-methoxy-2-methylsulfanyl-1*H*-pyrroles (R = Me, Et, *i*-Pr, *s*-Bu, *cyclo*-C_5H_9, *cyclo*-C_6H_{11}, Ph) lose methyl radical group from both methoxy and methylsulfanyl groups. The mass spectra of 1-*sec*-butyl- and 1-cycloalkylpyrroles also contained a strong peak (10–49%) from odd-electron $[M - C_nH_{2n}]^{+\cdot}$ ion formed via cleavage of the N–R bond with synchronous hydrogen transfer. Cleavage of the O–Alk bond in the fragmentation of 3-alkoxy-1-isopropyl-2-methylsulfanyl-1*H*-pyrroles (Alk = Et, *i*-Pr, *t*-Bu) was accompanied by rearrangement process leading to the corresponding alkene and odd-electron 1-isopropyl-2-methylsulfanyl-1*H*-pyrrol-3-ol ion. The main fragmentation path of 1-alkyl-2-methylsulfanyl-3-phenyl-1*H*-pyrroles (Alk = Me, *i*-Pr) under electron impact involves dissociation of the S–Me bond with formation of rearrangement 1*H*-[1]benzothieno[2,3-*b*]pyrrol-8-ium ion.

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