

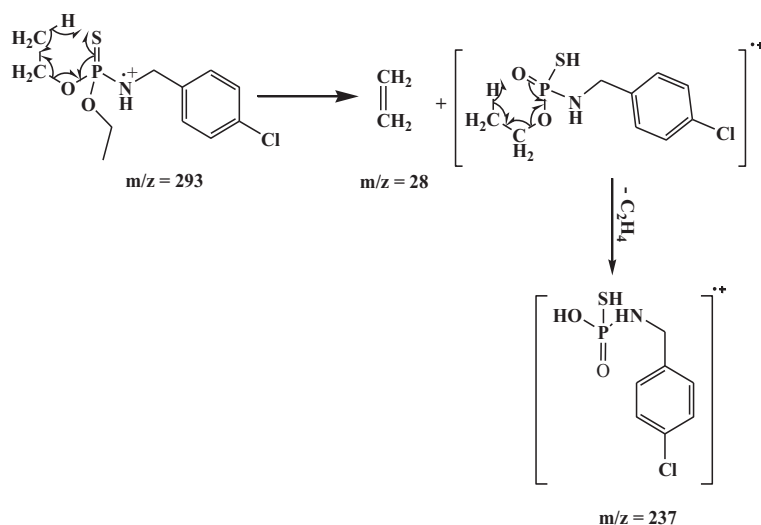
Mass Spectrometry Investigation of Some New Phosphoramidate and Thiophosphoramidate Compounds

Mehrdad Pourayoubi*, Mohammad Abad, Amir Hossein Alamdar, Ehteram Mohammadi Gooshki

Department of Chemistry, Faculty of Sciences, Ferdowsi University of Mashhad, Mashhad, Iran

(E-mail: pourayoubi@um.ac.ir)

In this research, some new phosphoramidate and thiophosphoramidate compounds were prepared from the reaction of amines with $P(O)Cl_3$ and $(C_2H_5O)_2P(S)Cl$ (commercial substances), 4- $CH_3-C_6H_4NHP(S)Cl_2$ (1), $((C_6H_5CH_2)(CH_3)N)P(S)Cl_2$ (2) and $CHCl_2C(O)NHP(O)Cl_2$ (3) (synthesized initial phosphorous-chlorine compounds). The compounds were studied by IR spectroscopy and mass spectrometry. In mass spectra, the fragmentation pathways and rearrangements are discussed. The formula of new compounds are as follows: (4- $CH_3-C_6H_4NH$) $P(S)(NHC_6H_4-3-Cl)_2$ (4), (4- $CH_3-C_6H_4NH$) $P(S)(NHC_6H_4-4-Cl)_2$ (5), $((C_6H_5CH_2)(CH_3)N)P(S)(NHC_6H_4-4-CH_3)_2$ (6), (4- $Cl-C_6H_4CH_2NH$) $P(S)(OCH_2CH_3)_2$ (7), $P(O)(NHCH_2C_6H_4-4-CH_3)_3$ (8), $(CHCl_2C(O)NH)P(O)(NHCH_2C_6H_4-4-CH_3)_2$ (9) and $(CHCl_2C(O)NH)P(O)(NHCH_2CH_2CH_3)_2$ (10). Mass spectra of all compounds 4, 5, 6, 7, 8, 9 and 10 show the ion molecule fragments, at m/z (intensity) = 421 (61), 421 (5), 395 (14), 293 (2), 407 (51), 413 (8) and 289 (11), respectively. The base peaks are as follows: for 4, 7 and 8 at m/z = 28, for 6 and 9 at m/z = 120 and for 5 and 10 at m/z = 126 and 150, respectively. The interesting rearrangement in mass spectrum of compound 7 is involved two McLafferty re-arrangement pathways (Scheme).



Scheme. The rearrangement in mass spectrum of compound 7 is represented.