Mass Spectrometry Investigation of Some New Phosphoramide and Thiophosphoramide Compounds

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In this research, some new phosphoramide and thiophosphoramide compounds were prepared from the reaction of amines with P(O)Cl3 and (C3H5O)2P(S)Cl (commercial substances), 4-CH3-C6H4NHP(S)Cl2 (1), (C6H5CH2)(CH3)N)P(S)Cl2 (2) and CHCl2C(O)NHP(O)Cl2 (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-CH3-C6H4NH)P(S)(NHC6H4-3-Cl)2 (4), (4-CH3-C6H4NH)P(S)(NHC6H4-4-Cl)2 (5), ((C6H5CH2)(CH3)N)P(S)(NHC6H4-4-CH3)2 (6), (4-Cl-C6H4CH2NH)P(S)(OCH2CH3)2 (7), PO(NHC6H4-4-CH3)2 (8), (CHCl2C(O)NH)PO(O)NHC6H4-4-CH3)2 (9) and (CHCl2C(O)NH)PO(O)NHC6H4-CH3)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).