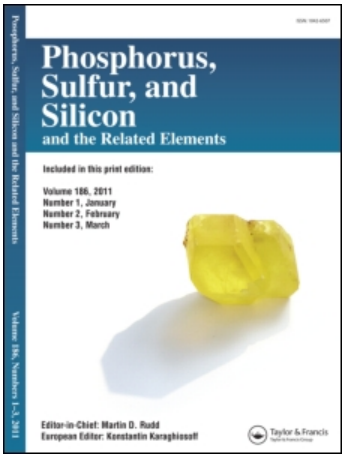

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The Positive and Negative Electrospray Ionization (ESI) Mass Spectrometry of 1-(*N*- Ethoxycarbonylamino) Arylmethylphosphonic Monoesters

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The Positive and Negative Electrospray Ionization (ESI) Mass Spectrometry of 1-(*N*-Ethoxycarbonylamino) Arylmethylphosphonic Monoesters

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The different mass spectrometric fragmentation of 1-(N-ethoxycarbonylamino) arylmethylphosphonic monoesters in positive and negative electrospray ionizations are briefly discussed.

Keywords 1-(*N*-ethoxycarbonylamino)arylmethylphosphonic monoesters; positive and negative mass spectrometry

1-Aminoalkylphosphonic acids are not only important phosphorus analogues of amino acids, but also one type of naturally occurring amino acid.[1] The positive and negative ion mass spectrometric fragmentations of 1-(*N*-ethoxycarbonylamino)arylmethylphosphonic monoesters have been investigated under electrospray ionization conditions. In the positive ion mass spectrometry, the protonated title compounds predominantly eliminate a phosphite monoester via a four-membered ring hydrogen rearrangement to yield protonated *N*-ethoxycarbonyl arylmethylimines as key intermediate fragment ions, which could further undergo four-, six-, or eight-membered ring rearrangements to produce mainly *N*-substituted/unsubstituted arylmethylimine ions.[2] It is interesting to note that the protonation of 1-(*N*-ethoxycarbonylamino)arylmethylphosphonic monoesters occurred in their arene rings. On the other hand, in the negative ion electrospray ionization (ESI) mass spectrometry, the

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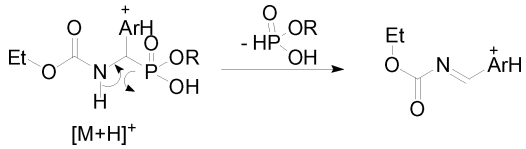
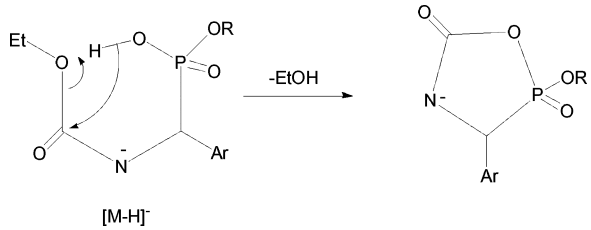
deprotonated title compounds favored to initially form phosphonic-carboxylic mixed anhydrides as the key intermediate fragment ions by loss of a molecular of ethanol, and they further eliminated CO or CO_2, respectively, to give rise to deprontonated three- and four-membered nitrogen and phosphorus containing heterocyclic fragment ions.



SCHEME 1 The initial positive-ion fragmentation pathway of the title compounds.



SCHEME 2 The initial negative-ion fragmentation pathway of the title compounds.

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[2] Y. Ma, W. Liu, and Y. Zhao, *Int. J. Mass Spectrom.*, **248,** 17 (2006).