脂肪胺分子离子及质子化脂肪胺分子的碎裂反应

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摘要 应用碰撞诱导解离(CID)

技术研究了电子轰击方法产生的脂肪胺分子离子和化学电离方法产生的质子化脂肪胺分子的碎裂反应。质子化脂肪胺碰撞活化后的主要碎裂通道包括丢失C~XH~2~X、C~XH~2~X~+~1、C~XH~2~X~+~2单元及NH~3和生成[C~yH~2~y~+~1]^+及CH~3CH=NH~2^+离子。脂肪胺分子离子碰撞活化后的主要碎裂通道是丢失C~XH~2~X、C~XH~2~X~+~1及NH~3和生成[C~mH~2~m~~1]^+、CH~2NH~2^+及CH~3CHNH~2^+离子。随着碰撞能的增加,

远电荷碎裂反应和电荷诱导碎裂反应之间竞争引起产物离子的分布发生变化,如[C~mH~2~m~~~1]^+和[C~yH~2~y~+~1]

^+离子。自由基机理可以解释质子化脂肪胺分子的远电荷反应。分子内氢抽取可以解释脂肪胺分子离子的碎裂反应。

关键词 质谱法 化学电离源质谱法 脂肪族胺 质子化作用 电子轰击 离子分子反应 碎裂反应 碰撞诱导解离

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Fragmentations of alkylamine molecular ions and protonated alkylamines

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Abstract The fragmentations of alkylamine ions C~nH~2~n~+~1NH~2^+ produced from 18 kinds of alkylamine salts by the electron impact ionization and protonated alkylamine C~nH~2~n~+~1NH~3^+ produced from them by the chemical ionization were examined using collision- induced dissociation. Major dissociation pathways of C~nH~2~n~+~1NH~3^+ include the loss of C~XH~2~X, C~XH~2~X~+~2, and NH~3, accompanied with the formation of [C~yH~2~y~+~1]^+ and CH~3CH=NH~2^+. Major dissociation pathways of C~nH~2~n~+~1NH~2^+ include the loss of C~XH~2~X~+~2, and NH~3, followed by the formation of [C~yH~2~y~+~1]^+, CH~2=NH~2^+ and CH~3CH=NH~2^+ and CH~3CH=NH~2^+. With increasing the collision energy, the distribution of the product ions was changed because of competing between the charge-remote fragmentation and charge-induced processes, such as [C~yH~2~y~+~1]^+ and [C~mH~2~m~~1]^+. The charge-remote fragmentation of protonated alkylamines and the fragmentation of alkylamine ions can be explaned by using the radical mechanism and hydrogen abstraction of intramolecule, respectively.

Key words MASS SPECTROGRAPHY CHEMICAL IONIZATION SOURCE MASS SPECTROMETRY ALIPHATIC AMINES PROTONATION ELECTRON BOMBARDMENT ION-MOLECULE REACTION FRAGMENTAION REACTION

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