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3-苯基-1-丁炔-3-醇质谱碎裂中[C8H7]^+的结构及分子内质子迁移反应

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摘要 报道了3-苯基-1-丁炔-3-醇的常规电子轰击质谱(EIMS)。利用碰撞诱导解离(CID)技术研究了质谱碎裂过程中产生的[C8H7]^+的气相离子结构。同时, 氘代同位素交换、亚稳(MI)和CID实验进一步证实了m/z 103离子的形成并不是分子离子的质谱碎裂中顺次失去甲基自由基和中性CO分子的直接氢迁移的协同反应,而是在失去CO分子前后发生了二次质子迁移反应的逐步过程。在此基础上提出了一种独特的双分子质子键合复合物中间体的碎裂机理。

关键词 质谱法 苯 P 醇 丁炔 P 碎裂 电子轰击质谱 迁移反应

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Structure of [C8H7]^+ and intramolecular proton transfer reactions in 3-phenyl-1-butyn-3-ol by MS/MS technique

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Abstract The electron impact mass spectrum (EIMS) of 3-phenyl-1-butyn-3-ol was reported in this paper. Collision-induced dissociation (CID) was used to study the gas phase ion structure of [C8H7]^+ formed by the fragmentation of ionized 3-phenyl-1-butyn-3-ol, and that it has the same structure as m/z 103 ions generated by cinnamic acid and α-methylstyrene. Deuterium labelling, metastable ion (MI) and CID experimental results indicate the formation of m/z 103 ion resulting from molecular ion of 3-phenyl-1-butyn-3-ol, which is a stepwise procedure via twice proton transfers, rather than concerted process during the successive elimination of methyl radical and neutral carbon monoxide accompanying hydrogen transfer. Moreover, in order to rationalized these fragmentation processes, the bimolecular proton-bound complex between benzyne and acetylene intermediate has been proposed.

Key words MASS SPECTROGRAPHY BENZENE P ALCOHOL BUTYNE P FRAGMENTATION TRANSLATION REACTION

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