

论文

小檗碱质谱碎片离子稳定性分析及碎裂机理的量子化学研究

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摘要:

用量子化学B3LYP/6-31G(d)方法, 研究了小檗碱质谱碎片离子的稳定性规律. 通过几何参数分析、结合能计算和前线分子轨道分析, 研究碎片离子可能的活性部位及各部位相对反应活性, 并从理论上探讨了质谱碎裂机理. 结合能计算结果表明, 分子离子中C9所连甲氧基的C—O键比C10所连甲氧基的C—O键更容易断裂. 同时发现, 质谱碎裂过程中, 氢的解离促进了羰基的解离, 即质谱中常见的解离CO的过程.

关键词: 小檗碱; 质谱; 量子化学; 碎片稳定性

Stability Analysis of Berberine Fragment Ions by Mass Spectrometry and Quantum Chemistry Studies on Fragmentation Mechanism

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Abstract:

Mass spectrometry and quantum chemistry DFT-B3LYP method were used to study the stabilities of berberine fragment ions. Binding energy was employed to study the activity of main radicals fragmented from the molecule. Theoretical methods including geometry parameter analysis as well as frontier molecular orbital analysis were combined to explore the possible CIDMS mechanism. It was shown that the methyl of C9 was more active than the methyl of C10, with a much smaller binding energy. Geometry parameter analysis confirmed that with the departure of hydrogen, it was easier for the carbonyl radical to leave from the molecule, which was in agreement with CID experiment.

Keywords: Berberine; Mass spectrometry; Quantum chemistry; Stability of fragment

收稿日期 1900-01-01 修回日期 1900-01-01 网络版发布日期

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#### 参考文献:

陈兰慧, 胡冬华, 王道武, 杨双阳, 苏忠民, 刘淑莹. 小檗碱质谱碎片离子稳定性分析及碎裂机理的量子化学研究. 高等学校化学学报, 2006, 27(5): 905-908

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