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论文

甲基丁烯醇的光电离实验与理论研究

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摘要:

利用同步辐射光电离质谱的方法研究了甲基丁烯醇($C_5H_{10}O$)在9.0~15.5eV的真空紫外光电离和光解离过程.通过测量光电离效率曲线,得到了$C_5H_{10}O$的电离能和主要碎片离子的出现势.通过对实验和计算结果的比较,分析了母体离子可能的光电离解离机理.母体离子的解离通道可以分为2类:由$C_5H_{10}O^+$直接发生键断裂的解离和经由过渡态的解离.确定了$C_4H^+_5$ 和$C_3H^+_5$离子的过渡态和中间体,其反应势垒与实验解离能是符合的.

关键词: 甲基丁烯醇 光电离和光解离 同步辐射 G3B3计算

Dissociative photoionization of methylbutenol: experimental and computational investigations

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Abstract:

Vacuum ultraviolet (VUV) dissociative photoionization of methylbutenol ($C_5H_{10}O$) in 9.0~15.5 eV was investigated with photoionization mass spectrometry using synchrotron radiation (SR). The ionization energy of $C_5H_{10}O$ and the appearance energies for the main fragment ions were determined with photoionization efficiency curves. The photodissociation mechanisms of methylbutenol were discussed based on comparison of our experimental results with those predicted by the quantum-chemical calculations. The dissociation channels may be divided into two types: the direct bond cleavage in $C_5H_{10}O^+$ and the reactions involving transition states. Transition states and intermediates for $C_4H^+_5$ and $C_3H^+_5$ were determined, and the reaction barriers were in agreement with the experimental dissociation energies.

Keywords: methylbutenol photoionization and photodissociation synchrotron radiation G3B3 calculation

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