Gas phase fragmentation of protonated esters in air at ambient pressure through ion heating by electric field in differential mobility spectrometry

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Abstract:
A planar differential mobility spectrometer has been used to study the ions formed at atm. pressure by a series of n-alkyl carboxylic acid esters (M). MH⁺ and M₂H⁺ ions were present at low temp. The combination of thermal energy and energy derived from collisional heating by acceleration in the asym. elec. field caused ion decompn. at an effective temp. (T_{eff}) higher than ambient. The products were the protonated carboxylic acids, F⁺. The elec. field thresholds for the first observation of F⁺ decreased as the temp. of the supporting gas atm. was increased and the rate, 1.5 °C per Townsend, was the same for all the esters. A measurable mass dependence for thresholds existed where the higher the molar mass for the ester of a given acid, the higher the required field. Although MH⁺ is the well-established precursor of the protonated acid, an apparent direct formation of F⁺ from M₂H⁺ was obsd. even though no MH⁺ was present in the spectrum. This is ascribed to T_{eff} being mass dependent. A field sufficient to raise a M₂H⁺ to T_{eff} for dissocn. to MH⁺ + M, raises MH⁺ to a higher T_{eff}, leading to its immediate decompn.