

THE APPLICATION OF A NITROGEN-COOLED ION MOBILITY TIME-OF-FLIGHT
MASS SPECTROMETER TO THE SEPARATION OF THE CONVENTIONAL AND
DISTONIC RADICAL CATIONS OF CH₃OH, CH₃NH₂, AND CH₃F.

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Ion mobility is an effective technique for separation of ions having differing electronic isomers. Here we describe the use of ion mobility time-of-flight mass spectrometry to separate conventional and distonic radical cations of CH₃X (X=OH, F, and NH₂). Both *ab initio* and density functional theory calculations have been performed to examine the structural differences of the conventional (CH₃X^{•+}) and distonic (CH₂[•]XH⁺) radical cations formed by electron impact from CH₃X (X=OH, F, and NH₂). In addition, we have employed variable temperature ion mobility to separate the isomeric ions. In this case separation is achieved on the basis of ion-neutral interactions between the ion and neutral buffer gas. We have also used computations and experiment to compare ion-neutral collision cross sections of the isomers based on calculated potential energy surfaces with the target gas. The results from our studies will be presented and compared to high level *ab initio* (MP2/6-311+G (d,p)) calculations.
