

# Electric Field Fragmentation of Mobility Selected Ions Using Tandem Ion Mobility Spectrometry at Ambient Pressure with Molecular Identification through Neural Network Analysis

---

Gary A. Eiceman, Hossein Shokri, Erkinjon Nazarov, Ben D. Gardner<sup>a</sup>, Hsein-Chi W Niu,<sup>a</sup> Gyoung-il Lee, John A. Stone

Department of Chemistry and Biochemistry, New Mexico State University, Las Cruces, NM 88003, <sup>a</sup>Collins Aerospace, San Dimas, California 91773

A tandem ion mobility spectrometer with a reactive stage at ambient pressure produced fragment ions from protonated monomers and established a foundation for molecular identification with ambient pressure technology. Fragmentation of alcohols was used as a model compounds to examine the formation of fragment ions in strong electric fields of mobility isolated ions with carbon numbers three to nine. Protonated monomers of individual alcohols were mobility isolated in a first drift region and were fragmented to carbocations at 64 to 128 Td and 45 to 89°C. Precursor and fragment ions were mobility characterized in a second drift region. Enthalpies for fragmentation of  $\text{ROH}_2^+$  to primary carbocations were calculated as 76 to 97 kJ/mole and enthalpies for subsequent charge migration to 2° carbocations were -49 to -58 kJ/mole. Spectra were also treated using backpropagation neural networks with training and testing of familiar and unfamiliar compounds. Findings suggest that much of the identification process could be attributed to memorization an about 30% learning on fragment ion patterns. In a bounded set of chemicals and five chemical families, classification and identification (both described as average adjusted values from the neural network) were greater than 0.95. Classification of unfamiliar compounds (those substances not used in any training or test of a network) showed rates over 0.5 for some compounds and others between 0.3 and 0.5. Increases of E/N to 150 to 200 Td should increase the amount of fragmentation and aid classification of unfamiliar compounds.