Spectral Analysis by Neural Networks for Compound Identification in Ion Mobility Spectrometry toward Small Tandem IMS Architectures

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Spectra from hand-held analyzers using ion mobility spectrometry (IMS) and operated in air at ambient pressure are often distinguished by relatively simple patterns including peak for ions derived from sample (M) through displacement reactions with hydrated protons per Equations 1 and 2:

$$H^+(H_2O)_n + M \dashrightarrow MH^+(H_2O)_{n-1} + H_2O \quad (1)$$

$$MH^+(H_2O)_m + M \dashrightarrow M_2H^+ + mH_2O \quad (2)$$

where n and m are often 2 to 4 with moisture from 10 to 100 ppm at 25°C. While the mobility coefficients for protonated monomers ($MH^+(H_2O)_m$) and proton bound dimers (M_2H^+) are characteristic of ion size and mass, little additional chemical information is accorded such spectra. The existence of fragment ions in ion mobility spectra can be seen in studies using neural networks where familiar and unfamiliar spectra were classified according to chemical family. In one study, a standardized database of 3137 spectra from 204 chemicals at various concentrations were assigned to ten chemical classes with 0.91 average success throughout a range of concentrations. Computational performance was matched between significantly different protocols at NMSU and UTAC. The region of the mobility spectrum containing fragment ions was determined empirically where these ions are located near K_o values of 1.8 $cm^2V^{-1}s^{-1}$ Although the mechanism or pathways for these fragmentation reactions is still under study, expected to involve energetic reactant ions that are promoted by low moisture in the supporting gas atmosphere. In a tandem IMS design, the protonated monomer and proton bound dimer will be isolated by mobility in a tandem drift tube and the isolated ion swarm fragmented in a strong electric field providing an increased level of specificity.