INTELLECTUAL MERITS

Gas phase ions in air at ambient pressure can 1) form stable clusters with polar neutrals and 2) can be fragmented through ion heating by strong electric fields. Such processes when introduced into ion measurements by ion mobility spectrometry (IMS) should significantly improve confidence of identification through added chemical orthogonality. This is best illustrated in tandem mobility determinations which have been demonstrated recently in an air atmosphere at ambient pressure. To experimentally address the introduction of chemical orthogonality into mobility analysis, we propose to develop a tandem instrument using planar differential mobility spectrometry (DMS) where ions, selected in a first mobility stage, can be fragmented with intense RF electric fields or can be clustered with a reagent gas, and then characterized by mobility in a next DMS stage. Each stage is 4 mm wide and 15 mm long. The results will provide the first ever systematic exploration of orthogonality in ion characterization by a combination of reagent chemistry and electric field strength. The results obtained from these studies will provide insights into the development of a next generation of hand-held analyzers used today in military preparedness, national security, and clinical diagnostics.

GOALS AND OBJECTIVES

The objectives of this project are to: 1) redesign and rebuild a proof-of-concept tandem DMS into a stable experimental platform, with detector options for a conventional Faraday plate or a mass spectrometer; 2) explore the selectivity of ion-reagent chemistry implemented in a tandem DMS and clarify origins of chemical orthogonality from changed alpha functions or ion transformations, and 3) determine chemical class-based dependences of ion fragmentation by strong RF fields in tandem mobility measurements.

Ion chemistry investigations will focus, with selected pharmaceuticals and pesticides, on the stability and mobility of clusters formed between sample ions and reagent gases. The importance of temperature, vapor concentrations, and moisture on chemical orthogonality will be determined. Orthogonality can be added through changes in strong electric fields and studies will disclose quantitatively the effect of field strength and ion structure on dissociation or fragmentation reactions. In a last accomplishment, improvements in selectivity through ion modification and the measurement value of chemical orthogonality will be determined in a triple stage DMS instrument.

BROADER IMPACTS

The proposed research utilizes concepts of measurements in mobility spectrometry which today is central to military preparedness and commercial aviation security. These methods have begun to impact clinical diagnostics and industrial process control. Students will develop proficiency in modern methods of chemical instrument design and construction and will develop familiarity with gas phase ion-molecule chemistry at ambient pressure. Since it is expected that the results from this research will provide measurement platforms useful to specific applications in industry or govenment, students will also develop familiarity with the presence of technology in society and the relationships to investigations outlined in this proposal. The PI will continue to actively involve undergraduate students in his research program, including undergraduate students from historically underrepresented groups, specifically the Hispanic, Native American and African American communities.