5. SIGNIFICANCE AND BROADER IMPACTS

5.1. Significance

The refinement of ion mobility spectrometry is relevant to issues of national security of the US and allied nations. Increasingly, IMS is being seen as a tool for high speed clinical diagnostics including therapeutic monitoring in lung disease. Lesser importance exists for industrial competitiveness (purity of gases, cleanliness of pharmaceutical production lines, and on-line monitoring of food/beverage production). All of these involve ambient pressure drift tubes and can benefit from improved resolving power. Tandem mobility instruments are a logical next advance in IMS and understanding the mechanisms by which chemical orthogonality can be introduced into these measurements is of interest for developing a next generation of chemical analyzers. Such analyzers should have chemistries/parameters configured for specific applications. Ion cluster formation and fragmentation are recognized as important factors in ion separations in DMS and ultraFAIMS. Although factors have not been specifically addressed in the context of tandem mobility measurements, it is likely that these factors will be important in introducing chemical orthogonality into mobility measurements and increase specificity and confidence of a measurement. The research outlined in this proposal intends to use substances of importance and systematic variations in structure with reagents spanning a range of moieties to build a broad understanding of specifics for chemical orthogonality. While our work will be modeled computationally in support of experiments, the studies outlined in this proposal will use an **experimental approach** to address the behavior of ions in vapor modified atmospheres and strong electric fields. To the best of our knowledge, this is **a unique experimental approach for chemical orthogonality in mobility measurements in any configuration and a first ever systematic exploration with tandem DMS.** It is likely that this experimental approach be applicable to studies on other mobility spectrometers and may affect the practice of mobility generally. The importance of this work is seen in a letter of support by a leading manufacturer of chemical instruments for security, Chemring Detection Systems, part of the ChemRing Group.

5.2. Broader Impacts

The proposed research utilizes gas phase ion molecule chemistry to improve measurements by chemical instrumentation. Students will develop proficiency in modern ion chemistry at ambient pressure, electronics, and software, and familiarity with mobility-mass spectrometry. Since it is expected that the results from this research will provide insights into the stability and structure of ion-neutral adducts as a function of gas temperature and heating by electric fields, students will also develop familiarity with computational chemistry and the relationships between these studies and measurement results in this proposal.

The PI has actively involved during 32 years 65 undergraduate, 52 MS level, and 15 PhD students in his research program. Currently, we have six undergraduate students currently constitute 25% of his research group. , and are coauthors on 26 of 186 (14%) of his independent publications. Current and former undergraduate students also include those from historically underrepresented groups, specifically the Hispanic, Native American and African American communities. The PI will continue to actively involve undergraduate students in his research program (funding has been requested to support undergraduate researchers). NMSU is classified as a minority serving institution (more than half of the students in the College of Arts and Sciences are self identified minorities).