PRF# 55183-ND6
Project Title: Electronic Spectroscopy of Organic and Organometallic Ions
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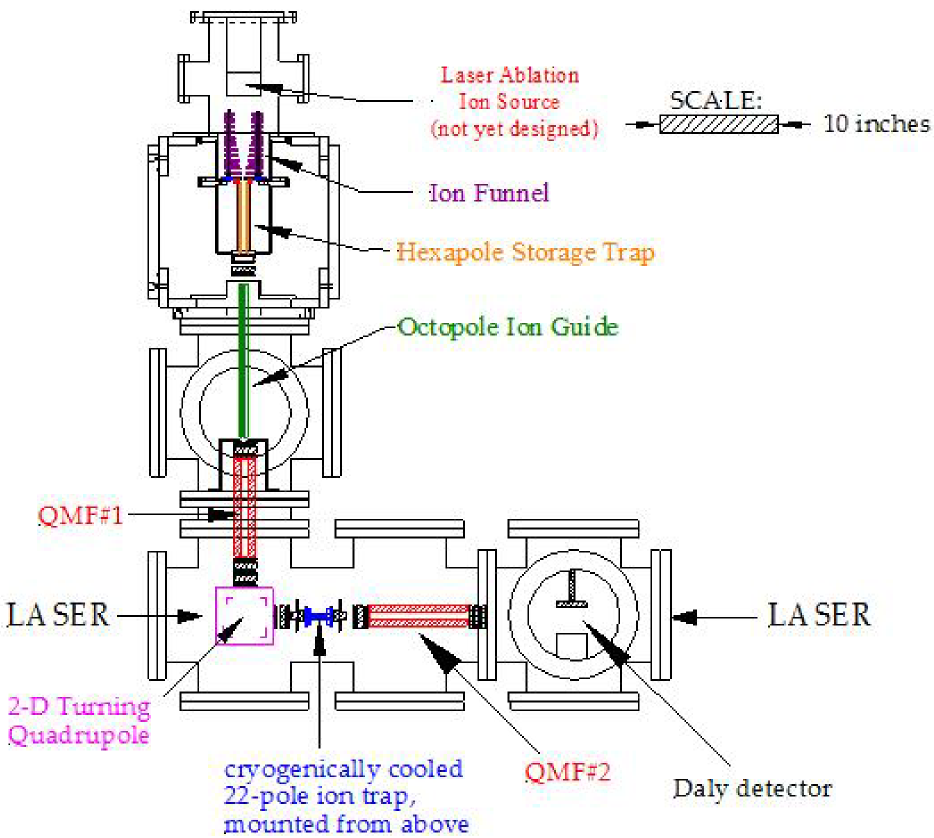
In this project, we seek to obtain electronic spectra of carbocations, including protonated benzene, alkenyl, dienyl, and trienyl cations, and acylium ions. These species are of interest as important intermediates in petroleum refining and reforming. We also seek to obtain electronic spectra of metal-methane addition adducts such as $H\text{-}M\text{-}CH_3^+$, $H_2M{=}CH_2^+$, $M{=}CH_2^+$, MH_2^+ and related systems in which an oxygen atom is included in the complex. These species are related to catalysts that can activate methane to form more useful products. Construction of our cryo-cooled ion photodissociation spectrometer was begun by my postdoctoral researcher, Sergei Aksyonov, who died unexpected on Sept. 11, 2015. The project was in limbo for about a year following Dr. Aksyonov's death. Since then, my graduate student, Jason Sorensen, and an undergraduate (now graduated), Erick Tieu, have worked to complete the construction of the instrument. A schematic of the instrument with modifications from the original design is shown below:



We have since discovered that the 22-pole trap is not optimal, because the ions are trapped in off-axis locations, where they are not irradiated by the photodissociation laser. We have designed and constructed a new trap based on an axial quadrupole design that will subject the trapped ions to a force that focuses them along the centerline. We anticipate that this will greatly increase the photodissociation yield of the trapped ions, but have not yet been able to test it because our electron-impact ion source required repair/redesign. While working on this, the electronic controller for one of our large turbopumps went out and is currently at the shop for repair. We have also designed and constructed an ion funnel/hexapole trap source to allow preliminary trapping of ions prior to injection into the first quadrupole mass filter. Again, this has not yet been tested because of the failure of the controller for the turbopump. This ion funnel/hexapole trap arrangement will be employed with various ion sources, including the laser ablation source, the electron-impact source, a glow discharge source, and an electrospray ion source. This work is providing invaluable training for my graduate student, Jason Sorensen, and for Erick Tieu, a former undergraduate in our department.

With the laser ablation ion source, we expect to produce several orders of magnitude more ions than can be produced with the electron impact source, allowing far greater numbers of ions to be trapped. This will also greatly increase the diversity of species that can be studied as compared to the electron impact ionization source, and will be needed for the studies of metal-methane reaction products.

When these modifications have been incorporated into the instrument, our first targets of study will be generated by electron impact of organic molecules, and will consist of protonated benzene, allyl cation, pentadienyl cation, heptatrienyl cation, and acylium ions. These will be followed by studies of metal ion-methane reaction products using the laser ablation source. We anticipate that completion of this instrument will open up a vast array of molecular ions for study, greatly expanding the scope of the PI’s research.