

Physical Chemistry Seminar

Tuesday,
February 4, 2014

11:00 am

Room 1315
Chemistry Building

Infrared Spectroscopy of Cold Ions and their Clusters: Inorganic and Organic Chemistry in the Gas Phase



Professor Michael A. Duncan

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Host: Professor Etienne Garand

Cold cations of metal-molecular complexes or of small hydrocarbons (aka "carbocations") are produced in a pulsed supersonic molecular beam by laser vaporization or pulsed discharge sources. These ions are mass-selected and studied with infrared photodissociation spectroscopy. Infrared spectra are compared to the predictions of theory (DFT and/or MP2) to elucidate the structures of these ions and, in the case of metal ions, their electronic states. Transition metal (Co, V, Mn, Cu) carbonyls or carbon dioxide complexes are studied in the C-O and CO₂ stretching regions. The spectra reveal coordination numbers, ligand vibrational shifts as a function of cluster size, and the occurrence of intracluster reactions. Ligand shifts compared to the predictions of density functional theory provide the spin state on the transition metal cation and how it changes upon progressive ligand addition. Carbocations (C₂H₃⁺, C₃H₅⁺, C₃H₃⁺, protonated benzene, protonated naphthalene) are studied in the C-H stretching and fingerprint regions of the spectrum. Several of these species exhibit more than one structural isomer, allowing investigation of the multiple minima on their potential surfaces. Unusual vibrations are detected for non-classical structures with bridging hydrogens. Protonated naphthalene has spectral lines relevant for the Unassigned Infrared Bands seen in interstellar gas clouds.

Refreshments will be available prior to the seminar at 10:45 a.m. outside room 1315

Graduate Students may meet with the speaker at 1:00 p.m. in Room 8335