Stony Brook University
The Graduate School

Doctoral Defense Announcement

Abstract

Vibronic Spectroscopy of the Cations of Substituted Benzenes and Time-of-Flight Mass-Spectrometry of Binary Metal Clusters Produced via Laser Ablation

By

Heather Alice Mann

Vibronic coupling in the cations of benzene and several monosubstituted benzenes was investigated using a variety of spectroscopic techniques. Mass Analyzed Threshold Ionization (MATI) spectroscopy was used to study the ground electronic states of Benzene cation, which is Jahn-Teller active. New pump-probe MATI spectra were obtained for both C6H6+ and C6D6+. These results, along with VUV-MATI results were compared to spectra simulated using a program that models the Jahn-Teller effect. Photo-induced Rydberg Ionization (PIRI) spectroscopy was used to examine the B states of benzonitrile, fluorobenzene and chlorobenzene cations. By using a variety of excitation schemes to obtain several complementary sets of MATI and/or PIRI data for each molecule, assignments can be made on the basis of symmetry selection rules. The monosubstituted benzenes have C2v symmetry and are therefore not Jahn-Teller active. Three excited states of the benzonitrile cation, however, lie very close together and it is interesting to see whether or not the higher two are coupling to the vibronic states of the lower. The frequencies observed were notably lower than calculated, indicating that the nearby electronic states are likely perturbing the B state. Vibrational frequencies were calculated for different electronic states of the cation and used to simulate the vibronic spectrum for this cation. In light of the success of the newly obtained Franck-Condon program, old experiments on fluorobenzene and chlorobenzene were re-evaluated.

Stoichiometries of binary metal clusters produced via laser ablation were studied using Time-of-Flight Mass-Spectrometry. The species examined are of interest in catalysis. The first species studied was the relatively small TiO molecule. The findings of the preliminary laser ablation experiment were used to assess its capabilities and limitations. These determined the types of experiments that would be possible with the facilities in our lab and then a more extensive experiment was performed on three families of molybdenum clusters, the carbides, nitrides and sulfides.

Date: August 7, 2007
Time: 10:00
Place: Chemistry, 410

Program: Chemistry
Dissertation Advisor: Philip M. Johnson