Announcing the Final Examination of Marjan Khamesian for the Degree of Doctor of Philosophy in Physics

Date: Monday, August 8, 2016
Time: 10:00 a.m.
Room: PSB 161
Dissertation title:
THEORETICAL STUDY OF NEGATIVE MOLECULAR IONS RELEVANT TO THE INTERSTELLAR AND LABORATORY PLASMA

Abstract:

Recently, several negative molecular ions, C_nN^- (n = 1, 3, 5) and C_nH^- (n = 4, 6, 8), were observed in the interstellar medium (ISM). It was suggested that the anions are formed in the ISM by the process of radiative electron attachment (REA). A simple statistical model was developed in 1980's to estimate rate coefficients of the REA reactions. Some of the rate coefficients obtained in the model are consistent with the observations, the others are not. More importantly, some of the approximations employed in the model are not physically based.

The aim of this thesis is a development of a quantum-mechanical approach to study the process of radiative electron attachment to linear molecules of astrophysical interest. The approach is based on first principles and accurate *ab initio* calculations of electronic bound and continuum states of the negative ion. Cross sections and rate coefficients for formation of the following molecular negative ions by REA were determined: CN^-, C_2H^-, C_3N^-, C_4H^-, C_5N^-, C_6H^- , and C_8H^-.
All the calculations presented in the thesis were carried out using the MOLPRO and UK R-matrix (Quantemol) suites of programs. Uncertainty quantification of the results, obtained for each studied system, was performed. The uncertainty of the final cross sections and rate coefficients were obtained by varying parameters of the computational model such as a chosen Gaussian basis set, the size of the R-matrix box, and other parameters of the model.

A second process, closely related to the radiative electron attachment, photodetachment (PD), was also studied in the thesis. PD cross sections for the CN^- , C_2H^- , C_3N^- , C_4H^- , C_5N^-, C_6H^-, C_8H^-, and C_2^- molecules were determined using an approach similar to the one employed for REA from the same transition dipole moment matrix elements. The obtained results were compared with available experimental PD cross sections. Good agreement with the experimental data was found. The obtained REA cross sections and rate coefficients were validated by comparing the present theoretical results with the experimental data from recent PD experiments.

Overall, given that the agreement between theoretical and experimental PD cross sections is good, the obtained REA cross sections are also correct. Therefore, the present results suggest that the observed abundance of these ions in the ISM can hardly be explained by the REA process. In other words, these anions are formed in the interstellar medium by a process different than radiative electron attachment.

Dissociative electron attachment (DEA) is another process of anion formation, which could possibly explain formation of certain molecular anions in the ISM. The ClF attachment was studied using a first principle approach: *ab initio* calculation of the ClF and ClF^- potential energy curves and R-matrix calculations were performed to determine the DEA cross section and rate coefficient. A good agreement with experimental data was demonstrated.

A theoretical approach to evaluate cross sections for rotational excitation of linear neutral molecules by an electron impact was developed and applied to acetylene, HCCH. The differential cross sections of HCCH were calculated for energies between 0.1 eV and 10 eV, and for transitions $j = 0 \rightarrow 0, 2, 4$. The momentum tr
calculated.

Outline of Studies:
Major: Physics

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M. S. Physics, University of Central Florida, USA, 2014
M. S. Particle Physics, University of Mazandaran, Iran, 2010

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Approved for distribution by Dr. Viatcheslav Kokoouline, Committee Chair, on August 2, 2016.

The public is welcome to attend.