

Chapter 8

Conclusion and Future Scope

Electron impact ionization of atoms and molecules is one of the most basic processes in physics, with fundamental applications in different areas like astrophysics, plasma physics, fusion physics, surface science, etc. Recent theoretical and experimental investigations have greatly contributed to the understanding of the scattering processes. Single and double differential electron emission cross sections are very vital in understanding the nature of the atomic and molecular state, and their interactions in nature. Sensitive nature of electron energy and angular distribution measurement puts several stringent requirements on the development of experimental setup. Moreover, the complexity of various excitation processes demands very advanced theoretical models to interpret the data. Complementary information on the mass of recoil ions generally improves the fidelity of the measurement but brings in its own stringent requirements. As one probe from atomic target to di or tri-atomic molecules the complexity in the measurements increases and this type generally titled as PEPICO for photon projectile and $e, 2e$ for electron impact, which grows substantially. This is mainly due to complex nature of molecular wavefunction and the requirement to capture the recoil ion mass as well as momentum information accurately to complete the picture. Thus the experimental setups for such measurements are quite elaborate and complex to design and build.

For larger molecules, the recoil ion momentum measurement becomes impractical due to their large mass and numerous fragmentation channels. But the electron emission cross-sections in correlation with mass brings in very elucidating details of the molecular properties. The main goal of the present work was to establish a system with capabilities to perform electron spectroscopy and recoil ion mass spectrometry in coincidence, specially tuned for large molecular targets. PAHs are the focus of this development due to their very intriguing behavior and their importance in nature. The astronomical significance of PAHs and PANHs can be assessed and understood only in the light of molecular structure and dynamics of individual PAHs or PANHs. The size of the family of PAHs

and PANHs compels us to perform molecular physics investigations on a few representative molecules and extend the understanding to the full spectrum of PAHs and PANHs. Considering large time scales of the order of millions of years, molecular dynamics is dominated by statistical dissociation processes. In such studies, it becomes extremely important to have an extensive quantum chemical structure calculation supported equally complex experimental apparatus.

As part of this work, an electron-ion coincidence experimental set-up was built. The development work involved full design fabrication and testing of the vacuum system and components hardware. Paralelly, full electronics, partly using modular electronics units off the shelf and partly by complete design and fabrication of vital electronics, was established. The pulsing techniques, as well as data acquisition for electron-molecule interaction with energy selective secondary electron-ion coincidence study, was then tested in various operational modes. The setup was then used to probe C_2H_2/HCN evaporation process in naphthalene and two of its nitrogen-containing derivatives under high-energy electron impact. These measurements were used to assess the rate of structural randomisation vis-a-vis HCN evaporation process. These results are of vital importance in understating the C_2H_2 and HCN population in ISM since they play an important role in astrobiological modeling. The results were complemented with the proton impact studies in the same velocity range. The results were compared to two ionizing modes, electron transfer, and electron emission mode. The work also took into account the plasmon contribution in all the cases.

8.1 Instrumentation and Setup Development

Setup was developed using SIMION8.0 simulations and the whole hardware was designed as a modular unit with high mobility and flexibility. This is needed since the full strength of the system can be realized with the angular distribution of the emitted electron measured using PSD. But this can be done only with photon impact which needs synchrotron radiation source (SRS). Hence the setup can be transported to an SRS beam line and can be used. The setup has several modes including a high mass resolution reflectron mode for

future use. A modular electron gun is built from cathode ray tube CRT of black and white television unit as an excitation source. Separate deflection and beam shaping electrodes are constructed by understanding the geometrical parameters from the simulation. The electron gun performance is tested with the different operation mode of the gun, afocal, broad, and zoom beam mode. In such type of e, 2e systems, the pulsing of high voltage plays a very important role. Hence two types of pulsing units were developed using commercial off the shelf power MOSFETs as part of this work. A single polarity high voltage pulser in which a pair of fast power MOSFETs triggered in synchronism for switching the electron beam ON or OFF was used. For the extraction of the molecular ion from the interaction region, a bipolar pulser is used which is a pair of switches working in synchronism but of opposite polarity. Both the switches were tested for the mass spectrometric and the possible electro-optic switching applications.

Multi-coincidence measurements invariably require a complex pulse processing and logic. Moreover, in this works the logic including the complex pulsing sequence of HV units to pulse the electron beam and pulse the mass spectrometer. The whole pulsing and processing sequence was realized as a part of this work. Moreover, the pulsing sequence was made modular to use the setup in different modes. A complete pulse processing and DAQ system were also developed as a part of this work.

8.2 Calibration and Testing

To understand the operating parameters the spectrometers were calibrated. For the calibration of CMA, the known Auger electrons were used, and the calibration graph was drawn for the detected electron as a function of the voltage applied to the CMA. The DDCS spectra of various atoms and molecules as a preliminary test. The position of Xenon secondary electron with a PSD at the focal point as well as away from the focal point of the CMA was shown to demonstrate the energy and angular distribution.

A similar calibration curve is drawn for ToF with Xenon ion, up to a charge state of Xe^{6+} . ToF spectra of various atoms and molecules are shown as the preliminary test results. The ToF unison with CMA was tested for the energy selective secondary electron-

ion coincidence measurement by using Xenon and naphthalene as the test sample.

8.3 Investigation of Structural Effects in Naphthalene and its Derivatives

The DEToF technique was implemented to investigate the time scales of fragmentation channels of the target molecules, and this technique is used to separate the fast and slow decay channels after electron impact. A detailed analysis of HCN loss showed identical time scales in quinoline and isoquinoline but nearly twice the yield in favor of isoquinoline. All these results were correlated with Arrhenius decay constant, internal energy and plasmon excitation energy.

Structural stability of this class of molecules is studied using electron as well as proton as the projectile by separating statistical and non-statistical decay channels. It is observed that in the case of electron impact at high velocity, as expected, the internal energy deposited to the molecule on an average is less and therefore the number of times C_2H_2/HCN loses is also decided by the structure, whereas structural alteration plays a very limited role. But in proton impact or at a lower velocity charge particle interaction, as expected, the internal energy deposited is more and therefore there arises more structural randomization. Now this work warrants even further exploration of a continuous variation of very low energy proton and very high energy proton as well as very low energy electron studies. To confirm this, due to practical difficulties, experiments could not be done with very high energy proton impact as well as very low energy electron impact, as both require a different machine. The metastable state of intermediate $C_8H_6^{2+}$ in naphthalene, quinoline and isoquinoline after C_2H_2/HCN loss was explored by using time-of-flight technique under proton impact. The similarities and differences in the structural properties of three molecules of PAHs and PANHs through theoretical calculation and a conclusion of the experimental results were drawn with the help of quantum chemistry calculation performed using HF method. This work has identified a method to study the structural randomization depending upon the internal energy of the molecule and a clear signature of the same has been seen in the case of naphthalene, quinoline, and

isoquinoline.

8.4 Future Scope

The electron-ion coincidence experimental set-up will be used with time-of-flight mass spectrometer in reflectron mode for mass resolution improvement. In addition, a parallel plate analyzer will be used for energy loss measurement of the projectile beam. By doing this kind of measurement we will be knowing the energy deposition to the target under charge particle collision and the following decay processes can be known. So a complete energetic study of the target molecule is possible. The experimental setup is made compact and modular, and it can be transported to facilities like synchrotron, high-energy ion source, free electron laser etc. for future experiments. For a complete understanding of PAHs and PANHs class of molecule, this study can be continued to other molecules apart from naphthalene and its two nitrogen derivatives. It will be a unique method and this work can be extended to more complex and important systems like biomolecules, aggregates, and clusters.