Electron induced dissociation of Pyrrole molecule

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Synopsis Comprehensive electron impact scattering study is carried out for pyrrole molecule focusing the dissociation by transient negative ion formation. Pyrrole is a biomolecule prototype of DNA components baring the great importance for an establishment of radiation damage model for living tissues.

Pyrroles are found in a variety of biological milieus, as parts of cofactors and natural products. Production of abundance of low energy electrons through high energy radiation leads to the single and double strand breaks in the DNA [1] is well established fact now. This has induced recent interest on electron-scattering studies in the investigation of biologically important compounds. High energy ionizing radiation is widely used in biomedical applications, both for diagnosis and treatment. In the low energy regime of the electron impact, incident electrons are captured by the target potential to form the shape resonance leading to the Dissociative Electron Attachment (DEA) Phenomenon [2-3]. This phenomenon is important from the point of view, eying the fragmentation and local chemistry of the targets. Discovery of DNA strand breaking by Boudaiffa *et.al.* [1] and striking experimental evidence that radiation damage could be mediated by DEA at low energies provided by Sanche and co-workers [4] have prompted us to take up the DEA studies of DNA and its prototypes. Thus, to design the radiation interaction model and to study the energy deposition in living matter, comprehensive data set for basic constituents of biological systems, from near thermal energy range (meV) up to very high (MeV) energies are well in demand. Since the unquestionable interpretation of data concerning electron-assisted processes with condensed bio-matter is difficult, accurate quantities describing particular electron collision events with biologically important compounds in gas-phase or with their simple analogues are very helpful. We have used R-matrix method [5-7] for low energy computation of eigenphases through which resonance width and resonant energy are computed which are important inputs for computing the DEA cross sections. Fig.1 presents the DEA cross sections for production of H^- anion. Peak at 12.62 eV shows the maximum probability of H^- production, which is supported by the broad shape resonance occurred at 12.22 eV with resonance width of 1.0267 eV. We have also observed

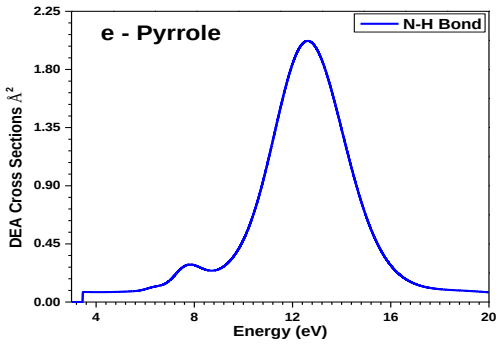

Figure 1. Dissociative Electron Attachment Cross Section for N-H bond in Pyrrole

numerous other resonances by eigenphase sum fitted to the Breit Weigner Profile [8]. Some of those may be attributed to the shape resonances causing the dissociative anions formation. In the present work we have studied the Pyrrole molecule comprehensively. Beginning from the target model establishment and target properties, various cross sections such as excitation, momentum transfer, differential and total cross sections are studied extensively. Detailed results will be presented at the time of conference.

References:

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