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Electron and positron scattering from pyridine

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Electron and positron scattering from pyridine

N Sinha[1]*, A K Sahoo[1] and B Antony [1]†

[1]Atomic and Molecular Physics Laboratory, Indian Institute of Technology (Indian School of Mines) Dhanbad, Jharkhand-826004, India

Synopsis Advancement in medical technology is a much needed demand in the present scenario. To stem a robust technology, one should be aware of the knowledge behind such sciences. In view of this, we investigate here the interaction of biomolecules with the most elementary particle, electron along with its anti-particle positron. The cross sections computed here using SCOP formalism for pyridine molecule will be useful for simulations of bio molecular systems. We further compare the cross sections for e^- and e^+ scattering extracting some rudimentary information about these basic interactions.

Over the last one and half decades, positrons have served as an important tool to diagnose human cell disorders through positron emission therapy (PET) and positherapy [1]. Consequently the investigation of interaction of positrons with various biomolecules is a requisite for its further investigation. Further, biomolecules are highly sensitive to radiation, causing damage arising from different reactive processes. These impairments may lead to cell death or carcinogenesis [1]. Hence, a precise study on the interaction of electron is vital to model these bio-molecular systems. The present study aims to calculate the interaction probabilities, more commonly known as the scattering cross sections, for both electrons and positrons. In addition a comparative study of the various cross sections for electron and positron would enhance our basic understanding of matter-antimatter physics. We intend to provide a comprehensive set of cross sections for pyridine (C_5H_5N), which is indispensable for Monte Carlo simulations of these bio-molecular systems. Note that these models require knowing such parameters over a broad energy range, in principle from the high incident energy of primary particles down to their final thermalisation in the medium. Besides, it allows estimating the transport properties in biologically relevant media.

Spherical complex optical potential (SCOP) [2] and complex scattering potential-ionization contribution (CSP-ic) [2] methods are employed for the computations of the cross sections for pyridine molecule. Since pyridine is a complex molecule, more than one scattering centre is identified. For each centre, a group is formed containing certain number of atoms. Based on the bond length and molecular structure, the charge density and static potential of each atom is expanded from this central atom. After obtaining the total charge density of the concerned group, we normalize the expression so that total number of electrons in the group is reproduced. Thus we obtain a spherical density and potential for each group, which is approximate, but it has a dependance on molecular properties as well. The cross sections obtained from each group is then added to give cross sections for the molecule. In case of positron scattering, positronium formation process is adequately included in the computations through a modified absorption threshold [2]. In the literature sufficient studies are available for electron scattering; however, for positrons the condition is poor. There is only one previous study [3] found for positron scattering cross sections, that too limited to 20 eV. The present work is aimed to produce cross sections for a wide energy range from 1 eV to 5000 eV for positrons and from 5 eV to 5000 eV for electrons. Hence, it is presumed that the present set of cross sections will contribute to the paucity of literature available and will be vital for the biomedical field.

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*E-mail: sinhanidhi00@gmail.com
†E-mail: bobby@iitism.ac.in