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Electron impact ionization cross sections of allene and propane molecules at low and high energy range

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Abstract. We have made a study of the total ionization cross sections of hydrocarbon molecules (allene, propane) due to electron impact for single ionization. Electron impact ionization cross sections (EIICS) have been calculated from threshold ionization energy to high energy (10 MeV). Along with EIICS calculation the values of collisional parameters are also calculated. The theoretical model, developed by Khare, has been modified to calculate the electron impact ionization cross section for molecules and atoms. The predicted EIICS of allene and propane molecules are compared with other theoretical and experimental data. Present model prevail a high degree of goodness of cross sections to the experimental data. Adequate comparisons of collisional parameter have been made with other available experimental values.

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Key words: ionization cross section, molecules, electron impact, collisional parameter

1 Introduction

The study of total ionization cross-sections by electron impact of molecules are required in the study of plasma diagnostics, astrophysical and fusion applications, radiation physics, mass spectrometry, ionization in gas discharge, modeling of fusion plasmas, modeling of radiation effects for both materials and medical research, and astronomy. Electron impact ionization cross sections (EIICS) at high energy have great importance in many accelerator applications. Cross sections due to ionization are needed for modeling of radiation effects in materials and in biomedical research and modeling of fusion plasmas in tokomaks. The computed data on

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cross sections are necessary in studying the problems of radiative association [1, 2]. Allene (C_3H_4) and propane (C_3H_8) are hydrocarbon molecules. Allene is the one of the isomers having the chemical formula C_3H_4 and others are propyne and cyclopropene. These isomers have different ionization potential. In our calculation we have used the isomer, which having the smallest ionization potential. The hydrocarbon molecules are one of the Earth's most important energy resources, and also an important part of the plasma processing. Currently hydrocarbons are the main source of the world's electric energy and heat sources.

Allene is chiefly used in organic synthesis. The EIICS for allene molecule have been calculated by Kim *et al.* [3] but no experimental data is available there. Kim *et al.* [3] theoretically calculated the total cross section for allene from threshold to 1 keV by using Binary Encounter Bethe theory. With best of our knowledge there is no experimental and theoretical data available for allene molecule at high energy range. For propane molecule the ionization cross sections have been calculated by Vinodkumar *et al.* [4] and Hwang *et al.* [5]. Hwang *et al.* [5] calculated the total cross section for propane from threshold to 1 keV by using Binary Encounter Bethe theory while Vinodkumar *et al.* [4] calculated from threshold to 2 keV. Vinodkumar *et al.* [4] calculated total cross section for elastic and inelastic collisions and total ionization cross sections are calculated by 'complex scattering potential-ionization contribution' method.

Propane is a nonrenewable energy source. It is used in semiconductor manufacture to deposit silicon carbide. Experimentally EIICS for propane is measured by various groups [6–10]. Measurement for propane is reported by Nishimura and Tawara [6], Schram *et al.* [7], Defrance and Gomet [8] and Duric *et al.* [9]. For high energy the electron impact ionization cross sections for propane have been measured by Reike and Prepejchal [10] from 0.1 MeV to 2.7 MeV.

One of the purpose of this work to calculate the electron impact ionization cross sections of the molecules by employing the useful features of Kim model [3] with Saksena model [11] to remove the deficiency of the later model at low energy. For CH_4 molecule Khare *et al.* [12] replaced $(1-\omega/E)$ by $(E'/E+U+I)$, where ω is the energy lost by the incident electron in the ionizing collision, E is the kinetic energy of incident electron, E' is the relativistic energy, I is the ionization energy, U is the average kinetic energy of bound electron. Here $U+I$ represent the increase in the kinetic energy of the incident electron due to its acceleration by the field of the target nucleus. In the present work we have extended Khare *et al.* [12] model to study the EIICS of allene and propane molecule in such a way that it yield better agreement between theory and experiments. To the best of our knowledge, this is the only theory which is applicable for such a wide energy range varies from threshold to several MeV.

2 Theory

Saksena *et al.* [11] have proposed a model for the molecular ionization cross sections. They started with the plane wave born approximation (PWBA) but later on included exchange and relativistic corrections. The transverse interaction through emission and the re-absorption