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Electron impact ionization cross sections of C_2H_2 and CH molecules at low and high energy range

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Abstract. In this communication, studies of the total ionization cross sections of hydrocarbon molecules (CH, C_2H_2) due to electron impact are presented. Electron impact ionization cross sections (EIICS) have been calculated from threshold ionization energy to high energy (10 MeV). Apart from EIICS calculation the values of collisional parameters are also calculated. The theoretical model, developed by Khare, has been modified to calculate the total ionization cross section for molecules. Obtained theoretical cross sections are compared extensively with a number of experimental and theoretical data. The obtained values of collisional parameter compared with the available experimental values.

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Key words: ionization cross section, C_2H_2 and CH molecules, electron impact

1 Introduction

The study 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 cross sections are necessary in studying the problems of radiative association [1, 2]. The hydrocarbon molecules are one of the Earth's most important energy resources, and also an important part of the plasma processing. Hydrocarbons are currently the main source of the world's electric energy and heat sources.

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Acetylene (C_2H_2) is used to volatilize carbon in radiocarbon dating which is widely used as a fuel and a chemical building block.

The EIICS for acetylene molecule electron impact ionization cross sections have been calculated by many researchers [3,4]. Kim *et al.* [3] theoretically calculated the total cross section for C_2H_2 from threshold to 1 keV by using Binary Encounter Bethe theory and 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. Experimentally total ionization cross section for C_2H_2 is measured by Zheng and Srivastava [5] for energy range threshold to 800 eV. For high energy the total cross section measured by Reike and Prepejchal [6] from 0.1 MeV to 2.7 MeV. For Methylidene (CH) molecule total ionization cross section measured by Tarnovsky *et al.* [7] for energy range threshold to 200 eV and calculated by Kim *et al.* [3] for energy range from threshold to 1 keV while Vinodkumar calculated up to 2 keV. For CH there is no experimental and theoretical data available for high energy range according to best of our knowledge. Experimentally total cross section for high energy range is available for acetylene only by Reike and Prepejchal [6].

One of the purposes of this work to calculate the electron impact ionization cross sections of the molecules by employing the useful features of Kim model with Saksena model to remove the deficiency of the later model at low temperature. For CH_4 molecule Khare *et al.* [8] replaced $(1-\omega/E)$ by $(E'/E'+U+I)$, where ω is the energy lose suffered by 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 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.* [8] model to study the EIICS of CH and C_2H_2 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.* [9] 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 of the virtual photons along with the longitudinal interaction through the static unretarded coulomb field are also included. However, PWBA requires continuum generalized oscillator strengths (CGOS), which are very difficult to evaluate. Hence, they employ a semi-phenomenological relation of Mayol and Salvet [10] which expresses CGOS in terms of the continuum optical oscillator strengths (COOS). The use of the above relation breaks the expression of the ionization cross-section σ_j for the j^{th} molecular or-