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Total ionization cross sections of NO_2, CO and CS molecules due to electron impact

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Abstract. The total cross sections for NO_2, CO and CS have been calculated by Binary-Encounter-Bethe [BEB] method of Khare from threshold energy to 10 MeV due to electron impact. This model has been developed by combining the useful features of Plane Wave Born Approximation (PWBA) and BEB model of Kim. It is shown that Bethe and Mott cross section terms differ from those of the Kim [BEB] method but their sums are very close to other. Results are presented with the help of graphs. Adequate comparisons of collisional parameter have been made with other available experimental values. The calculated cross-sections are compared extensively with a number of all possible experimental data and theoretical results.

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Key words: ionization cross section, molecules, electron impact

1 Introduction

Total ionization cross-sections of molecules by electron impact 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 [1], etc. NO_2 is an atmospheric pollutant, founds in troposphere and stratosphere. Nitrogen dioxide plays a role in atmospheric chemistry, including the formation of troposphere ozone. In plasma physics, ionization of NO_2 plays important role [2]. CO plays a major role in modern technology, in industrial processes such as iron smelting and as a precursor to myriad

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products. CS is also present in atmosphere. These molecules are important constituents that found at different altitudes of the atmosphere [3].

For these molecules experimentally the total ionization cross sections have been measured by various groups Lindsay *et al.* [4], Lukic *et al.* [5], Lopez *et al.* [6], Freund *et al.* [7], Hudson *et al.* [8] and theoretically calculated by Kim *et al.* [9] and Joshipura *et al.* [10]. Total cross sections for NO_2 are measured by Lindsay *et al.* [4], Lukic *et al.* [5] for energy range threshold to 1 keV whereas Lopez *et al.* [6] measured it for energy range threshold to 2000 eV. Kim *et al.* [11] used Binary-Encounter-Bethe [BEB] model to calculate total ionization cross section. Total cross sections for CO are measured by Mangan *et al.* [12], Hudson *et al.* [8], for energy from threshold ionization energy to 250 eV. However Rieke and Prepejchal [13] have measured the total cross section in the energy range 0.1 MeV to 2.7 MeV. Freund *et al.* [7] have measured the partial ionization cross sections for CS for threshold to 200 eV. According to best of our knowledge for NO_2 and CS there are no experimental data and theoretical cross sections available for high energy range. Kim *et al.* [9] have used Binary Encounter Bethe theory with the vertical ionization potential to calculate the total cross section. Joshipura *et al.* [10] have calculated the total ionization cross sections by using 'complex scattering potential-ionization contribution' method.

In 1997 Saksena *et al.* [14] proposed a model for the molecular ionization cross sections by using the plane wave born approximation (PWBA) which includes transverse as well as longitudinal interactions. They have employed the exchange and relativistic corrections. In PWBA continuum generalized oscillator strengths (CGOS) are required, which are very difficult to evaluate. Hence, they employed a semi-phenomenological relation of Mayol and Salvet [15] 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 orbital into two terms one representing the Bethe term (Soft collision) and other one the Mott term (hard collision). Later on this model was modified by Khare *et al.* [16] for CH_4 molecule, where $(1-\omega/E')$ was replaced by $E'/(E'+I+U)$, where ω is the energy lose suffered by incident electron in the ionizing collision, E' is the relativistic kinetic energy of incident electron, I is the ionization energy, U is the average kinetic energy of bound electron. Here $I+U$ represent the increase in kinetic energy of the incident electron due to its acceleration by the field of the target nucleus. Furthermore, they have employed the useful features of the Binary Encounter Bethe models of Kim and Rudd [11]. Following Kim *et al.* they have used the COOS $df/d\omega = NI/\omega^2$ and dropped the contribution of exchange to Bethe term. They have also shown that Bethe and Mott cross-section terms obtained by Kim *et al.* are the approximate forms of their model. Although Bethe and Mott cross-sections in Khare *et al.* model are different corresponding cross-sections of Kim [BEB] model but the total ionization cross sections obtained in both model are very close to other. In Khare *et al.* [BEB] method calculated cross sections were in better agreement with the experimental data over a wide energy range varying from threshold to several MeV.