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TOTAL (ELASTIC + INELASTIC) CROSS SECTIONS FOR ELECTRON SCATTERING FROM N_2O, CF_4, NO AND F_2 MOLECULES

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Electron impact total (elastic + inelastic) cross sections and total ionization cross sections are calculated for N_2O, CF_4, NO and F_2 molecules from the thresholds to 5 keV. A model complex optical potential is calculated for each collision system from the corresponding molecular wave function at the Hartree-Fock level. The resulting complex optical potential, free from any adjustable parameter, is treated exactly in a variable-phase approach to calculate scattering complex phase shifts and the total cross sections. The present results are found to be consistent with the existing experimental measurements.

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Keywords: electron scattering, elastic scattering, inelastic scattering, total cross sections, total ionization cross sections

1. Introduction

Electron scattering by atoms and molecules is of fundamental importance in a great variety of physical and chemical processes and thus its determination has been a subject of continuously increasing interest for both experimentalists and theoreticians working in this field [1]. The study of electron scattering by N_2O, CF_4, NO and F_2 molecules have important application in space, atmospheric physics, plasma, laser and chemical physics [2]. The design of plasma reactor is still based on empirical studies due to lack of reliable cross sections for the excitation and dissociation pathways in reactive gases employed in plasma processing.

It is to be noted here that the well-known independent-atom model (IAM) [3] for intermediate and high-energy molecular scattering is suitable for elastic scattering only [4]. In the IAM procedure, the molecular behavior is included only via the internuclear geometry, while the true nature of the molecular charge distribution is missing. At this time, a spherical complex optical potential (SCOP) method appears to be reliable and practical technique of predicting σ_t values for a large variety of molecules [5].

In the SCOP method, the spherical part of the complex optical potential is treated exactly in a partial-wave analysis to yield cross-section parameters. The neglect of non-spherical terms in the full expansion of the optical potential is based on the fact that such an anisotropic contribution is very small in the intermediate- and high-energy regions. In the present work, we have calculated basically the electron impact total cross sections σ_t for N_2O, CF_4, NO and F_2 molecules at incident energies almost from the threshold of electron excitation to 5 keV. We have also estimated the total ionization cross sections σ_i from total inelastic cross sections and compared with available experimental results. The present calculations are based on the complex optical potential approach and use of variable phase approach method [6].

2. Theory

The interaction of the electron-molecule system can be represented by a local complex optical potential

$$V_{\mathrm{opt}}(r) = V_{\mathrm{R}}(r) + \mathrm{i}V_{\mathrm{abs}}(r)\,, \tag{1}$$

where, the real part is a sum of three parts

$$V_{\mathrm{R}}(r) = V_{\mathrm{st}}(r) + V_{\mathrm{ex}}(r) + V_{\mathrm{pol}}(r)\,. \tag{2}$$

The static potential $V_{\mathrm{st}}(r)$ is calculated from the unperturbed target wave function ψ_0 at the Hartree-Fock level. The term $V_{\mathrm{ex}}(r)$ accounts for electron exchange interaction, while the $V_{\mathrm{pol}}(r)$ represents approximately the short-range correlation and long-range polarization effects. In this energy region, a local potential model for exchange and polarization is adequate.

$V_{\mathrm{abs}}(r)$ is the absorption potential. First we determine the target charge density $\rho(r)$ of a given molecule,

$$\rho(r) = \int |\psi_0|^2 dr_1 dr_2 \cdots dr_Z = 2\sum_{\alpha} |\phi_\alpha(r)|^2\,, \tag{3}$$

where, Z is the number of electrons in the target, ϕ_i is the i^{th} molecular orbital and a factor of 2 appears due to spin interaction, and α is the sum over each doubly-occupied orbital. It can be shown that for closed-shell molecules, $\rho(r)$ belong to a totally symmetric one-dimensional irreducible representation of the molecular point group [7]. All four potential terms (V_{st}, V_{ex}, V_{pol}, and V_{abs}) are functions of $\rho(r)$.

For example,

$$V_{\mathrm{st}}(r) = \int \rho(r_1)|r - r_1|^{-1} dr_1 - \sum_{i=1}^{M} Z_i |r - R_i|^{-1}. \tag{4}$$

The $V_{\rm ex}$ is the Hara free-electron-gas-exchange (HFEGE) model [8] and $V_{\rm pol}$ is calculated in the correlation-polarization (COP) approximation [9 – 11]. Thus, the accurate evaluation of $\rho(r)$ is important in our SCOP model. We employed various single-centre expansion programs to determine the charge density and various potentials for linear and nonlinear molecules. The molecular polarizabilities α, which are used to calculate the polarization potential, are given in Table 1.

The imaginary part of the optical potential $V_{\rm abs}$ is the absorption potential, which represents approximately the combined effect of all inelastic channels. Here we employed a semi-empirical absorption potential as discussed by Truhlar and co-workers [12]. The absorption potential is a function of molecular charge density, incident electron energy and the mean excitation energy Δ of the target.

$$V_{\rm abs}(r) = -\rho(r)\left(\frac{\nu_{\rm loc}}{2}\right)^{1/2}\left(\frac{8\pi}{5k^2k_f^3}\right) \times H(k^2 - k_f^2 - 2\Delta)(A_1 + A_2 + A_3)\,, \quad (5)$$

where,

$$\nu_{\rm loc}(r) = k^2 - V_{\rm st}(r) - V_{\rm ex}(r) - V_{\rm pol}\,, \quad (6)$$

$$A_1 = \frac{5k_f^3}{2\Delta}\,, \quad (7)$$

$$A_2 = -\frac{k_f^3(5k^2 - 3k_f^3)}{(k^2 - k_f^2)^2}\,, \quad (8)$$

$$A_3 = \frac{2H(2k_f^2 + 2\Delta - k^2)(2k_f^2 + 2\Delta - k^2)^{5/2}}{(k^2 - k_f^2)^2}\,. \quad (9)$$

Here $\frac{1}{2}k^2$ is the energy of the incident electron, k_f the Fermi momentum and $H(x)$ is the Heaviside function, $H(x) = 1$, for $x \geq 0$, and $H(x) = 0$ for $x < 0$. By varying the value of Δ in $V_{\rm abs}$, one can improve the absorption $\sigma_{\rm abs}$ or $\sigma_{\rm t}$ cross sections relative to experimental or more accurate *ab initio* calculations. In our calculations, we have fixed Δ to be the ionization potential (I.P.) of the molecule since the calculated value of Δ is very close to the ionization energy in most of the molecules.

The molecular properties used in the calculations are shown in Table 1.

After generating the full optical potential of a given electron-molecule system, we treat it exactly in a partial-wave analysis by solving the set of first-order coupled differential equations for the real and imaginary parts of the complex phase-shifts function under the variable phase approach (VPA) [13].

To obtain the total ionization cross section $\sigma_{\rm i}$, a semi-empirical approach is applied to derive it from the calculated $\sigma_{\rm abs}$. The total inelastic cross section $\sigma_{\rm inel}$ or $\sigma_{\rm abs}$ may be partitioned as

$$\sigma_{\rm abs}(E_i) = \sigma_i(E_i) + \sum \sigma_{\rm exc}(E_i)\,, \quad (10)$$

with $\sigma_{\rm i}$ the total cross section for all allowed ionization processes and $\sum \sigma_{\rm exc}$ the sum over total excitation cross sections for all accessible electronic transitions. The

TABLE 1. Molecular properties used in the calculations of total (elastic + inelastic) cross sections for electron scattering from N_2O, CF_4, NO and F_2 *molecules.*

Molecule	Z	I.P.(eV)	$\alpha(a_0^3)$
N_2O	22	12.89	20.23
CF_4	42	14.7	19.06
NO	15	9.264	11.46
F_2	18	15.697	7.11

second term arises mainly from low-lying dipole-allowed transitions for which the cross section decreases rapidly at high energies. The quantity $\sum \sigma_{\rm exc}$ becomes less important than $\sigma_{\rm i}$ at energies well above the ionization threshold [14]. The inelastic cross sections $\sigma_{\rm inel}$ or absorption cross sections $\sigma_{\rm abs}$, which are a quantities not accessible directly in experiments, can be partitioned basically as Eq. (10). The first term stands for all the allowed ionization processes in the targets by electron impact. The ionization corresponds to infinitely many open channels, so that as incident energy increases above the ionization threshold ($\sim$ 10 eV), the ionization cross section $\sigma_{\rm i}$ provides the major contribution to the theoretical quantity $\sigma_{\rm inel}$ or $\sigma_{\rm abs}$. We have estimated the ionization cross section $\sigma_{\rm i}$ from our calculated inelastic cross sections $\sigma_{\rm inel}$. The second term is the sum of the total excitation cross sections for all accessible electronic transitions. These transitions are dominated by low-lying dipole allowed states, for which the thresholds lie below the ionization energy ($\sim$ 10 eV). We have not calculated the excitation cross sections at such low energies. The contribution of excitation cross sections is very small above 100 eV.

We have obtained the electron-impact total (elastic+inelastic) cross sections $\sigma_{\rm t}$ and ionization cross sections $\sigma_{\rm i}$ for molecular targets N_2O, CF_4, NO and F_2 at energies $E_{\rm i} \geq 10$ eV. Although the present study is unable to provide directly the electron-impact total ionization cross sections. The total absorptions cross sections $\sigma_{\rm abs}$ which account for all inelastic contributions including both excitation and ionization processes. It was concluded by Lee et al. [15] that ionization dominates the inelastic process about 70 − 80% at energies around 100 eV and about 100% for energies above 300 eV. The estimated ratio of $\sigma_{\rm i}$ to $\sigma_{\rm abs}$ is roughly about 0.7, i.e

$$\frac{\sigma_{\rm i}}{\sigma_{\rm abs}} = 0.7\,. \tag{11}$$

In the present work we have calculated the electron-impact ionization cross sections using $\sigma_{\rm abs}$ and compared with available experimental data.

3. *Results and Discussion*

We have obtained the electron-impact total (elastic+inelastic) cross sections $\sigma_{\rm t}$ and ionization cross sections $\sigma_{\rm i}$ for molecular targets N_2O, CF_4, NO and F_2 at energies $E_{\rm i} \geq 10$ eV.

Figure 1 represents our theoretical σ_t and σ_i for $e^- -$ N_2O scattering along with measured data. The present σ_t is agree with the experimental measurement of Kwan et al. [16] above 100 eV. Our calculated σ_t is overestimated by about 5 to 10%

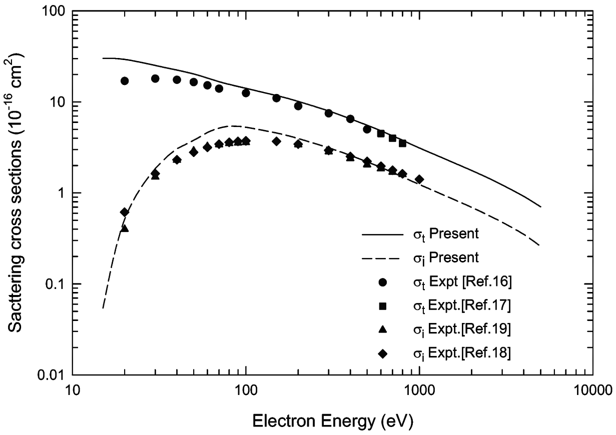

Fig. 1. Electron scattering by N_2O *molecule.*

near 20−50 eV. The experimental σ_t of Xing et al. [17] are in good agreement with present results. On comparing our estimated σ_i with experimental measurements of Rapp and Englander-Golden [18] and Iga et al. [19], the calculated σ_i is overestimated about 10% near intermediate energies because other inelastic channels are open near this energy range. In general, good agreement is found between our calculated σ_i and experiments for energies above 200 eV, where the absorption effects are expected to be important.

Figure 2 presents results of $e^- -$ CF_4 scattering. Our calculated σ_t is compared with available integrated elastic measurements σ_{int} of Boesten et al. [20] and Sakae

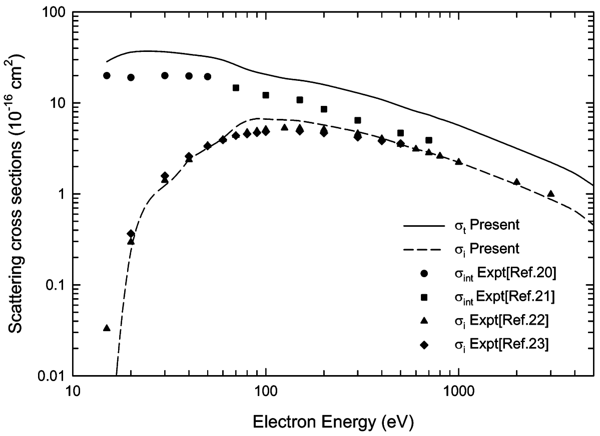

Fig. 2. Electron scattering by CF_4 *molecule.*

et al. [21]. We are also notice that σ_{int} values lie below the σ_{t}. We reproduce the shape of σ_{t}. This provides good estimation of our calculated σ_{t}. The present σ_{i} is compared with experimental measurements of Nishimura et al. [22] and Ma Ce et al. [23]. Our calculated and experimental data agree in the entire energy range. The overestimation near 100 eV of about 5% due to other inelastic processes.

Figure 3 represent $e^{-}-$ NO scattering. Our calculated σ_{t} is compared with experimental data of Szmytkowski and Maciag [24]. Our present results overestimate $10-15\%$ than experiment below 100 eV. The present σ_{i} are in good agreement with experimental measurements of Rapp and Englander-Golden [18] and Lindsay et al. [25] at all energies.

Figure 4 shows our calculated σ_{t} and σ_{i} for $e^{-}-$ F_2 scattering. No experimental measurements are available in literature for comparison. The shape of curves of the total cross sections and total ionization cross section are reproduce here.

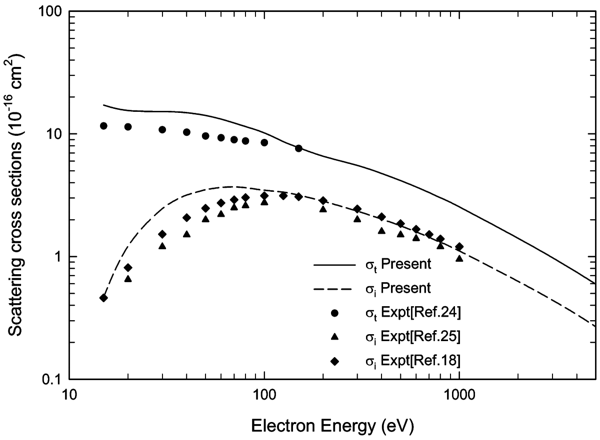

Fig. 3. Electron scattering by NO *molecule.*

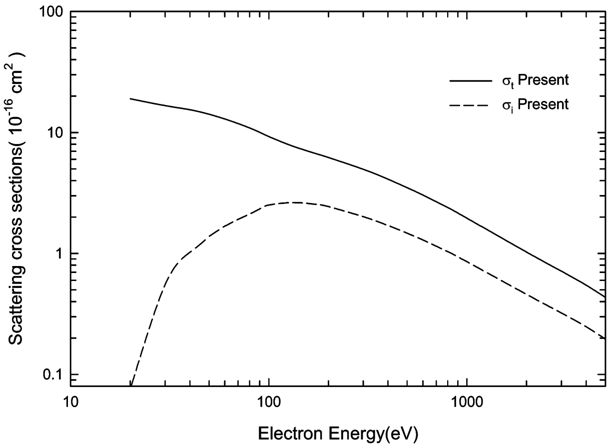

Fig. 4. Electron scattering by F_2 *molecule.*

4. *Conclusions*

We have presented the total (elastic + inelastic) and total ionization cross sections of the intermediate and high energy electron impact. A complex optical potential is derived for each system from target wave functions and its spherical part is employed to yield total cross sections under the complex phase-shifts analysis. We have avoided any kind of fitting procedure in the present calculation. The present model mainly requires the target charge density, polarizability, ionization potential etc. of the molecule. At and above 100 eV, our results for all the molecules studied here are in good agreement with available measurements. The method employed here is easy and practical and requires no prior information on the cross section parameter.

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UKUPNI (ELASTIČNI I NEELASTIČNI) UDARNI PRESJECI RASPRŠENJA ELEKTRONA NA MOLEKULAMA N_2O, CF_4, NO I F_2

Izračunali smo ukupne elektronske sudarne (elastične i neelastične) i ukupne ionizacijske udarne presjeke za molekule N_2O, CF_4, NO i F_2 za energije od praga do 5 keV. Modelske kompleksne optičke potencijale smo izračunali za svaki sustav na osnovi odgovarajućih molekulskih Hartree-Fockovih valnih funkcija. Postignute optičke potencijale, bez parametara za podešavanje, primijenili smo egzaktno s promjenljivim fazama u računima kompleksnih faznih pomaka i ukupnih udarnih presjeka. Ishodi računa su u skladu s dostupnim rezultatima mjerenja.