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Electron scattering from molecule CH_4 at 10–5000eV *

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Electron scattering from molecules in the intermediate- and high-energy range is investigated employing the developed semi-empirical formula for electron scattering from diatomic molecules. Total cross sections of e-CH_4 scattering are obtained over an incident energy range of 10–5000eV. The results agree well with other available experimental and theoretical data. According to our formula, some quantitative information of single Yukawa potential are also obtained.

Keywords: total cross sections, bond length, Yukawa potential
PACC: 3410, 3480

1. Introduction

Considerable attention has been devoted to the electron scattering from molecules because the scattering process is closely related to several practical applications and molecules have some special structure. For example, CH_4 possesses a tetrahedral symmetry and can be regarded as spherical in the process of investigation. So the relative simplicity in the theoretical treatment of electron scatterings from molecules enables the testing of different models and forms of electron–target interactions. In this paper we are interested in the e-CH_4 collision in the intermediate- and high-energy range. Although a large number of experimental[1−5] and theoretical works [6−8] have been done, quite large discrepancies remain in the determination of characteristic features of the $\sigma(E)$ curves.

Relations between total cross sections and physical-chemical parameters of target molecules may indicate the role of some microscopic properties in the scattering process and should be described by a semi-empirical formula which may help to estimate the total cross sections of electron scattering by target molecules. In recent years, total cross sections for electron scattering have been measured for families of targets in order to study the variation of total cross sections for different targets, such as simple hydrocarbon molecules,[3] methyl halides [9] and isoelectronic ($N_E = 18$) molecules.[10] Nishimura and Tawara [3] established a correlation between the magnitude of total cross section and the geometrical size of the target for a group of simple hydrocarbons at intermediate energies. Floeder *et al*[9] confirmed the correlations between the total cross section and the number of electron in the molecule. The formula reflecting the total cross sections, electron impact energy and target polarizability had been proposed and used.[3] Zecca *et al*[11] used a fit formula to fit the total cross sections of some molecules, considered that one fit parameter has relationship with bond length of some hydride molecules (such as NH_3, CH_4, H_2O, H_2S and SiH_4), but they did not give out the quantitative dependence on the parameter. Recently, March *et al*[12] analysed total cross sections for electron scattering on "quasi-spherical" molecules (CH_4, SiH_4 and GeH_4) over a wide energy range. Simple analytical formulae ($E\sigma$=constant) was presented at low and high energies and could be derived from quantum scattering theory. We also obtained a semi-empirical for-

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mula for total cross sections of electron scattering from diatomic molecules,[13] which reflects the quantitative dependence of the total cross sections on the nuclear distance of the diatomic molecules, and we have developed it for some simple hydrocarbon molecules.

In this paper, total cross sections for electron scattering from CH_4 are calculated employing the developed semi-empirical formula over an incident energy range of 10–5000eV. In section 3, we also obtain some quantitative information of single Yukawa potential according to our formula. The final concluding remarks are made in section 4.

2. The developed semi-empirical formula and results

We have obtained a semi-empirical formula for total cross sections of electron scattering from diatomic molecules.[13] Here we will give a brief outline of the semi-empirical formula for completeness, and include further details which have not been discussed in our earlier works.

Utilizing the energy dependence in the Born approximation ($\sigma_T(E) \to AE^{-1}$, if $E \to \infty$), and analysing a large number of experimental and theoretical data, we find that the following formula for total cross sections of electron scattering by molecules in the intermediate- and high-energy range is suitable

$$\sigma_T(E) = \frac{d\sigma_0}{d + C\sigma_0 E}, \qquad (1)$$

where E is the collision energy of the electron in eV; d(Å) and σ_0(Å^2)are two free parameters for a particular molecule, which can be fitted by two points of energy and the corresponding total cross sections.

Let $C = 10^{-3}$(eVÅ)$^{-1}$. By using formula (1) and the experimental data of some special systems, such as e-CO, e-N_2, e-NO, e-O_2 and e-HCl, we find $d \approx 2r_0$. This implies that the total cross section of electron scattering by a diatomic molecule depends on the internuclear distance r_0. In formula (1), σ_0 is the total cross section which corresponds to zero impact energy. If we treat the electron–molecule interactions as a "hard sphere" potential with radius r_0, the total cross section of zero impact energy would be equal to $4\pi r_0^2$.[15] Let $d = 2r_0$ and $\sigma_0 = 4\pi r_0^2$. We obtain an alternative semi-empirical formula:

$$\sigma_T(E) = \frac{4\pi r_0^2}{1 + C2\pi r_0 E}. \qquad (2)$$

In contrast to the diatomic molecules, CH_4 has a trigonal pyramidal shape, and the maximum scale along the bond axis between the constituent atoms equals to the bond length r_0. Therefore, we set $d = 2r_0$ and also treat the interactions of electron with CH_4 roughly as a "hard sphere" potential with radius of r_0 for Eq.(1), which neglects their long-range interactions of electron with CH_4 in this paper. So we hold that formula (2) for total cross sections of electron scattering by CH_4 in the intermediate- and high-energy range is appropriate.

Using formula (2) and values of r_0=1.093Å[15] for CH_4, we have calculated the total cross sections of electron scattering from CH_4 in the 10–5000eV energy range. For the comparison with available experimental data,[1–5] recent calculation by using the optical potential model and additivity rule[7] and SCOP results of Jain and Baluja[6] are shown in Fig.1.

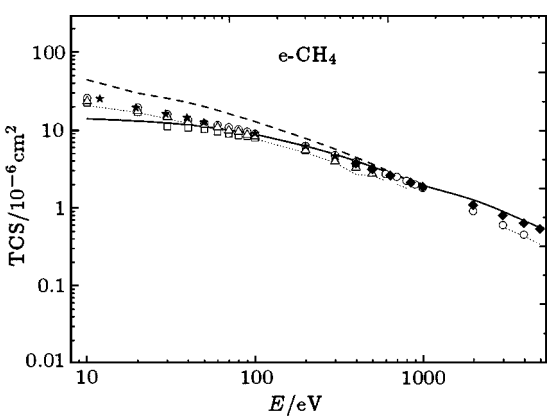


Fig.1. Total cross sections of e-CH_4 scattering: solid curve, from formula (2); dashed curve, Ref.[7], dotted curve calculated, Ref.[6], experimental data: stars, Ref.[1]; squares, Ref.[2]; circles, Ref.[4]; triangles, Ref.[3]; diamonds, Ref.[5].

From Fig.1, we note that the present total cross sections of e-CH_4 obtained from semi-empirical formula (2) agree well with the experimental data[1–5] above 40eV. The results also agree well with the data of recent calculation[7] above 200eV. In the range of 40–200eV, the results agree well with the SCOP results of Jain and Baluja,[6] and the SCOP results only agree with the experimental data [3] and lower than the experimental data[1,2,4,5] above 200eV.

The discrepancies remain in Fig.1. This is because that we treat the interactions of electron with CH_4 roughly as "hard sphere" potential with radius of r_0. This approximation only considers the short-range interactions of electrons with CH_4 and neglects

the long-range interactions. The leading term of the long-range interactions is $-\alpha_0/r^4$ (α_0 is the polarizability). For non-polar molecules, the next important long-range term is the dynamical effects in the dipole polarization interaction. Since the long-range interactions are different from each other, so the discrepancies in Fig.1 still remain.

3. A simple Yukawa potential with the bond length

The Yukawa potential was proposed as a model for the nucleon interaction on the basis of meson theory by Yukawa:

$$V(r) = -\frac{V_0}{r}\mathrm{e}^{-\frac{r}{a}}. \tag{3}$$

It also appears in atomic and molecular physics as a simple model potential for the e-atom or e-molecule collisions. However, the Yukawa potential, as a model for the nuclear interactions that has been most extensively investigated, has not been obtained sufficient information, especially quantitative information on the strength (V_0) and the range of (a) of the molecular scattering potential. Zecca *et al*[11] found that the total cross sections can be well approximated by a single or a double Yukawa potential. They also obtained quantitative information on strength (V_0) and the range (a) of some molecular scattering potential, but the values of V_0 and a rely on the experimental data. If we treat the e-molecule interactions as a single Yukawa potential, then the total cross section can be well described by the formula [16]:

$$\sigma_T(E) = \frac{4\pi V_0^2}{a^2\left(a^2 + \frac{2mE}{\hbar^2}\right)}. \tag{4}$$

Comparing Eq.(1) with Eq.(4), we can gain the magnitudes of a and V_0,

$$a = \sqrt{\frac{m}{C\pi r_0 \hbar^2}}, \tag{5}$$

$$V_0 = \frac{m}{C\pi\hbar^2}. \tag{6}$$

Eq. (5) shows that the applicable range of the single Yukawa potential depends on the bond length of CH_4. From Eq.(6), we can find that the strength of the single Yakawa potential is a constant, and does not depend on the physical-chemical parameters of CH_4.

4. Conclusions

Our developed semi-empirical formula has yielded encouraging results for the total cross sections of the e-CH_4 collision system. The formula definitely reflects that the total cross sections of e-CH_4 collision depend on the bond length of CH_4. Though the semi-empirical formula cannot present very exact solutions, the results can provide a quantitative, good comparison and foretell the results for experimental research, particularly for those molecules for which no theoretical calculations can be done. According to our formula, we also obtain some quantitative information of the single Yukawa potential, which with the bond length does not reflect the interaction of electrons with CH_4 accurately, for the semi-empirical formula neglects the long-range interactions.

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