

Elastic Scattering of Low Energy Electrons by Hydrogen Molecule

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Abstract The coherent version of the Renormalized Multiple-Centre Potential Model (RMPM) has been extended to treat the elastic scattering of low energy electrons by H_2 molecule. In the present study, the Intramolecular Multiple Scattering (MS) effect has also been included. The comparison against the experimental data shows that the inclusion of the MS improves significantly the agreement with experiment. The extension of the present method to study electron-polyatomic molecule interaction is also discussed.

1. INTRODUCTION

The electron scattering by gaseous atoms and molecules has been a subject of considerable theoretical and experimental investigations during the past decades¹⁻³.

Particularly in the low impact energy region (below the first ionization threshold), considerable progress has been made. In this energy range only few reactive channels are open and therefore sophisticated *ab initio* formulations are computationally feasible; hence, they have been widely applied to study electron linear-molecule and electron-atom scattering successfully^{4,5}.

Nevertheless, even in the low energy range the study of collision processes by *ab initio* methods is very expensive in computer time and therefore a formidable computational effort will be required to extend these theoretical methods to an energy range above the first ionization threshold. This fact drastically limits the overall applicability of *ab initio* methods.

On the other hand, model potential approaches have been proposed to study the electron-molecule interaction, particularly in the inter-

mediate and high energy range. Among them, the coherent version of the RVM (Renormalized Multicentre Potential Method), proposed by Lee and Freitas⁶⁻⁸ has been applied to calculate Differential Cross Sections (DCS) for elastic and vibrationally inelastic processes in electron-molecule collisions at intermediate energies.

The RVM formalism was extended (Jain *et al.*^{9,10} and Botelho *et al.*^{11,12}) by the inclusion of the intramolecular Multiple Scattering (MS) effects into the electron-molecule collision dynamics. Results from the RVM and RVMMS calculations are encouraging when compared against experimental measurements and other theoretical data.

In the present paper the applicability of the RVMMS approach in the low energy range is investigated through the study of the electron-Hydrogen molecule scattering at 7-15 eV impact energies.

The RVM theory has already been described in detail by Lee and Freitas⁶⁻⁸ and the general formulae for the cross sections with the inclusion of the Multiple-Scattering terms can be found in articles of Hayashi and Kuchitsu¹³ and Jain and Taya¹⁴.

In section 2 we briefly present some of the RVM fundamental equations and in section 3 our results and conclusions will be reported.

2. THEORY

In the optical potential model the effective electron-molecule interaction potential can be written as

$$V_{\text{int}} = V_{\text{st}} + V_{\text{Ex}} + V_{\text{pol}} \quad (1)$$

where V_{st} , V_{Ex} and V_{pol} are respectively, the static, exchange and polarization contributions to the electron-molecule interaction potential.

In the RVM approximation the static contribution is given by:

$$V_{\text{st}} = \sum_{\alpha=1}^N V_{\text{st}}^{\alpha} + V_{\text{st}}^{\text{MC}} \quad (2)$$

with

$$V_{st}^{\alpha}(\vec{r}) = -\frac{Z_{\alpha}}{r} + C_{\alpha} \sum_i^{OCC} \int \frac{\rho_i^{\alpha}(\vec{r}; \vec{R})}{|\vec{r}-\vec{r}_0|} d\vec{r}_0 \quad (3)$$

where Z_{α} is the atomic number of the α 'th atom in the molecule C_{α} is a charge renormalization constant and ρ_i^{α} is the electronic charge generated by the i -th occupied molecular orbital. V_{st}^{MC} is a non-spherical part of the potential resulting from the delocalizing of the electronic charge density (due the formation of chemical bonding) and belongs to the same point group symmetry of the molecule. Therefore, in the RVM formalism all the terms in equation (2) can be generated from the molecular wavefunction.

In the present work the polarization potential, V_{pol} is assumed to have the adiabatic form proposed by Henry and Lane¹⁵.

Finally the contribution of the exchange effect is included through the energy-dependent free-electron-gas approximation suggested by Hara¹⁶.

The Rosen¹⁷ Hydrogen molecule wavefunction was used to generate the charge density distribution which is needed for the static and exchange potential calculations.

A partial wave analysis was performed to evaluate the phase-shifts and the DCS was obtained in the framework of the Adiabatic Nuclei Approximation, as discussed in our earlier papers.

As the DCS experimental data are not rotationally and vibrationally resolved, our theoretical values were obtained by performing the summation over all the rotational and vibrational levels of the hydrogen molecule through the technique of closure, which leads to a final DCS values averaged over the orientations of the molecule.

3. RESULTS AND DISCUSSION

In figures 1-3 our present theoretical results are compared against absolute experimental measurements of Shyn and Sharp¹⁸ and Nishimura et al¹⁹.

One can observe that the agreement between theoretical and experimental results improves as the electron impact energy increases. The

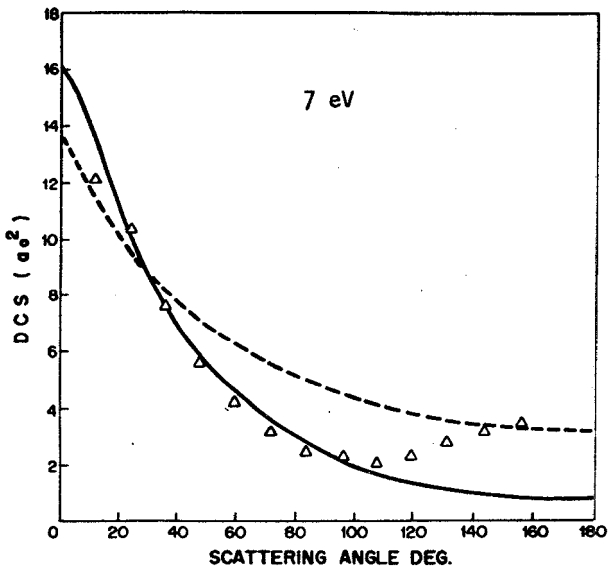


Fig.1 - Elastic Differential Cross Sections (DCS) for Electron-Hydrogen Molecule Scattering. — RMPM+MS; --- RVFM; Δ Exp. Shyn and Sharp¹⁸.

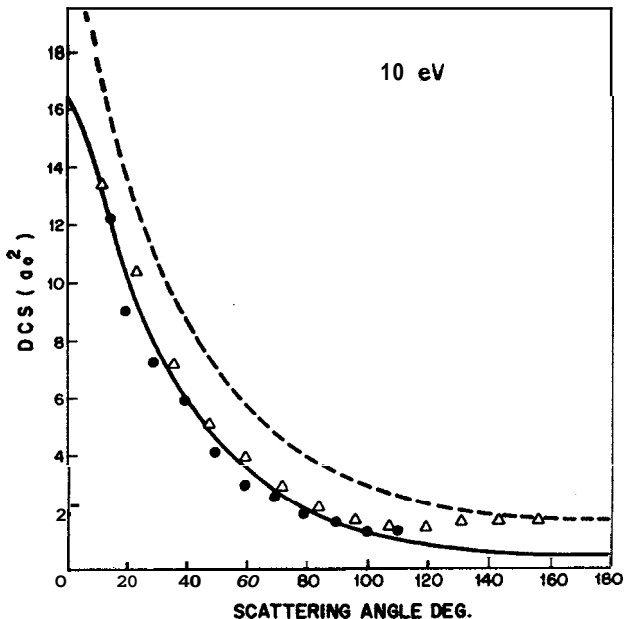


Fig.2 - Elastic Differential Cross Sections (DCS) for Electron-Hydrogen Molecule Scattering. — RMPM+MS; --- RVFM; Δ Exp. Shyn and Sharp¹⁸; ● Exp. Nishimura et al¹⁹.

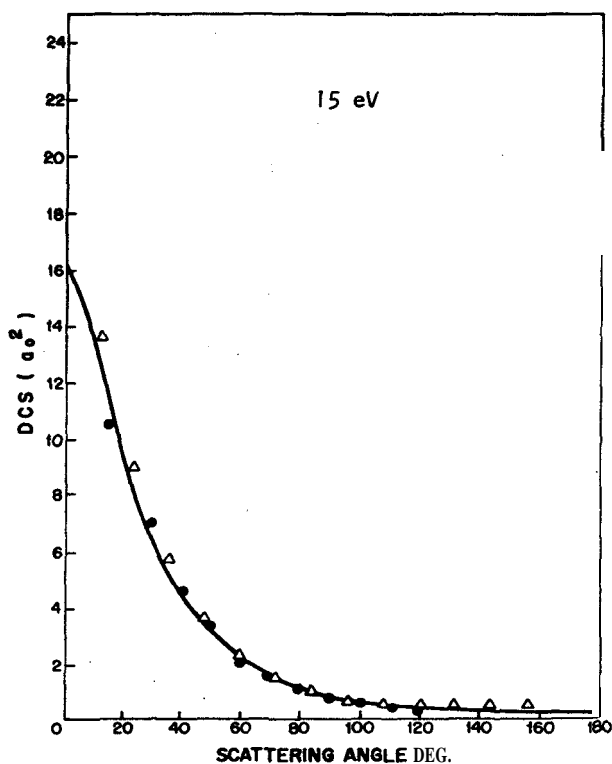


Fig.3 - Elastic Differential Cross Sections (DCS) for Electron-Hydrogen Molecule Scattering. — RMPM+MS; Δ Exp. Shyn and Sharp¹⁸; ● Exp. Nishimura et al¹⁹.

inclusion of intramolecular multiple scattering effects significantly improves our calculated DCS. A similar achievement was also found in the earlier work of Botelho et al¹¹ and Lee et al¹².

However, approaching the low energy limit, our theory is not able to reproduce the experimental DCS at large scattering angles.

This discrepancy can be attributed to the fact that, in the present work, higher terms in the multipole expansion of the non-spherical part of the electron-molecule interaction potential were neglected and probably also due to the truncation of the intramolecular Multiple Scattering series, which has been included in the present work only up

to second order (double scattering). The contributions of the higher order terms might be significant at lower energies.

An overall analysis of the present results clearly demonstrates the need of introducing Multiple-Scattering effects to obtain the DCS in agreement with experimental data.

The good agreement between our theoretical DCS with the experimental data in a wide range of scattering angles ($0-100^\circ$) is indicative of a possible applicability of the RVMMS approach in the study of electron-molecule scattering at low energies.

Particularly, a possible extension of the present formalism to include electron scattering by non-linear molecules is also encouraging. In these cases, corrections to take into account higher terms in the multipole expansion of the electron-molecule interaction potential and related contributions to the intramolecular Multiple Scattering effects could be included through the distorted-wave approach.

Another important question to be investigated is connected to the fact that, at low energy the collision process is more sensitive to the details of the potential surface and consequently to the quality of the wavefunction used to generate the molecular charge density.

These investigations are in progress and will be reported later.

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Resumo

A versão coerente do Modelo do Potencial Multicêntrico Renormalizado (MPMR) com a inclusão do Espalhamento intra-molecular (EI) é estendida para o estudo do Espalhamento elástico de elétrons de baixa energia pela molécula de H_2 . A comparação com as medidas experimentais mostram que a inclusão do EI melhora sensivelmente a concordância entre os resultados calculados e experimentais. A possibilidade do presente método ser estendido ao estudo da interação de elétrons com moléculas poliatômicas é também discutida.