Rotational excitation of methane molecule by electron impact

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Abstract— *Electron scattering by methane molecule plays a crucial role in understanding the interaction dynamics between electrons and molecules. In this research, we focus on investigating the elastic and rotational excitation process for electron scattering by CH_4 within the energy range of 5-30 eVThe main objective is to calculate the differential and total cross sections to provide insights into the scattering behavior and energy transfer mechanisms involved in these collisions.*

To achieve this, advanced theoretical model and computational method are employed. Accurate potential energy and interaction potentials specific to CH_4 are utilized to ensure reliable and precise calculations. The calculated cross sections are compared with experimental data and previous theoretical studies to validate their accuracy and assess the effectiveness of the computational approach. The results obtained from the calculations of the differential and total cross sections shed light on the angular distribution of the scattered electrons, the potential energy governing the electron-molecule interaction, and the rotational dynamics of CH_4 molecule during electron collisions. These findings contribute to a comprehensive understanding of electron-molecule interactions and have implications in various scientific disciplines. The research provides a comprehensive investigation of electron scattering by CH_4 and offers valuable insights into the underlying physics of elastic and rotational excitations. The calculated cross sections serve as fundamental inputs for theoretical models and simulations, enhancing our ability to predict and interpret experimental observations. The outcomes of this study contribute to the broader field of electron-molecule interactions and pave the way for further advancements in this area of research.

Keywords— *electron scattering, methane molecules cross sections, rotational excitation, energy transfer, potential energy.*

I. INTRODUCTION

The investigation of electron scattering by molecules has provided valuable insights into the fundamental processes of electron-molecule interactions. Understanding the elastic and rotational excitation cross sections for electron scattering by CH_4 molecule is of great significance in elucidating the scattering dynamics and energy transfer mechanisms involved in these collisions[1]. In earlier works, Hassan and Khalaf[2, 3].investigate the excitation of atoms by electron impact .Lately we work an the scattering of electrons interacting with NH_3 and PH_3 molecules[4] , and the stopping power of electrons interacting with NH_3 and other molecules[5]. In this study,

we aim to calculate the differential and total cross sections for elastic and rotational excitations of electron scattering by CH_4 molecule within the energy range of 5-30 eV.The elastic scattering cross section quantifies the probability of electrons undergoing non-reactive collisions with CH_4 , where energy is exchanged between the electron and the molecule without inducing any permanent changes in its structure. By calculating the elastic scattering cross section, we can investigate the angular distribution of the scattered electrons, the potential energy surfaces governing the electron-molecule interaction, and gain insights into the collision mechanisms[6]. These results contribute to a

comprehensive understanding of electron-molecule interactions in CH_4 systems[7].

In addition to elastic and rotational excitation cross sections provide crucial information about the rotational dynamics of CH_4 molecule upon electron collisions. Rotational excitation occurs when the electrons transfer sufficient energy to induce transitions between different rotational energy levels in the molecule[8]. The calculation of rotational excitation cross sections enables us to determine the probabilities of various rotational transitions and examine the rotational energy transfer processes occurring during electron-molecule collisions [9]. To compute the differential and total cross sections for elastic and rotational excitations in electron scattering byCH_4, advanced theoretical models and computational methods have been employed[6, 10-13]. The calculated cross sections will be compared with available experimental data and previous theoretical studies to validate their accuracy and assess the effectiveness of our computational approach.

The outcomes of this study have wide-ranging implications in various scientific disciplines. The obtained cross sections contribute to a deeper understanding of electron-molecule interactions; provide essential inputs for plasma diagnostics, astrochemical modeling, and atmospheric chemistry studies[14] . Moreover, these results facilitate the development of comprehensive scattering models, improving our ability to predict and interpret experimental observations[15] .The structure of this paper is organized as follows: Section 1 is Introduction; Section 2 will provide an overview of the theoretical framework and computational methods used in this study. Section 3 will present and discuss the computed differential and total cross sections for elastic and rotational excitations in electron scattering by CH_4 within the energy range of 5-30 eV. These results will be discussed in comparison with available experimental data and previous theoretical studies .finally Section 4 is the Conclusions.

II.   THEORETICAL FORMULATION

In order to calculate the rotational excitation cross sections for electron scattering by methane molecule and determine the differential and total cross sections, a theoretical framework is employed. This framework utilizes advanced computational methods and theoretical models specifically designed to accurately describe electron-molecule interactions[7].

To characterize the scattering process, expressions for the scattering amplitude in the body-fixed (BF) frame of reference are utilized. These expressions were derived by Gianturco and Thompson in 1980[16]. The scattering scenario considers methane as a rigid rotor, allowing for spherical, symmetric, or asymmetric rotational motion. The scattered electron wave function is obtained by solving a set of inhomogeneous coupled differential equations that govern the rotational excitation process and describe the transition from the initial level to the final level.

In any quantum mechanical description of atomic particles, the fundamental Schrödinger equation encompasses an interaction Hamiltonian and the associated wave function of the entire system.

$$(\mathcal{H} - \mathrm{E})\psi_T(r,R) = 0 \qquad (1)$$

Where the e^- molecule Hamiltonian is given by

$$\mathcal{H} = \mathcal{H}_e(r) + V_{int}(r,R) + \mathcal{H}_m(r) \qquad (2)$$

Here $\mathcal{H}_e(r)$ is the kinetic energy term for the projectile, $\mathcal{H}_m$ is the Hamiltonian of the isolated molecule (R represents both electronic and nuclear coordinates), $V_{int}(r,R)$ is the interaction (Couiombic) operator between the electron and the molecule, E is the total energy of the system and 0T is the total eigenfunction of the e^- molecule system.

In elastic Scattering the expression for the DCS (Diffrential cross section) of a generic polyatomic molecule as follows:[17]

$$\frac{d\sigma}{d\Omega} = \sum_L A_L P_L \cos\theta \qquad (3)$$

The expression involves the Legendre function $P_L(cos\theta)$ A_L coefficients given before in [17]. The essential T-matrix, in turn, is defined as a function of the S and K-matrices.

$$\boldsymbol{T_{lv,l'v`} = \delta_{ll`}\delta_{vv`} - S_{lv,l'v`}} \qquad (4)$$

$$\boldsymbol{T_{lv,l'v`} = 1 - (1 - iK_{lv,l'v`})(1 + iK_{lv,l'v`})^{-1}} \qquad (5)$$

The integral cross section is expressed as follows:

$$\boldsymbol{\sigma^T = \frac{\pi}{K^2}\sum_{lv}\sum_{l'v`}\left|T_{lv,l'v`}\right|^2} \qquad (6)$$

In the case of symmetric top molecules, the expression for the$\frac{d\sigma}{d\Omega}$ A_L coefficients is provided in[17].

$$\frac{d\sigma}{d\Omega}\left(J_T - J'_{T'}\right) = \frac{k'}{k}\sum_L A_L\left(J_T \rightarrow J'_{T'}\right)P_L(\cos\theta) \qquad (7)$$

$$\boldsymbol{A_L(Jk \rightarrow J`K`) = \frac{(2j+1)(2L+1)-1^L}{4K^2}\sum_{ll'IP} i^{l-l'}\,[(2l+1)(2l'+1)(2l`+1)(2l'`+}$$
$$\boldsymbol{1)]^{1/2} X\binom{l`\ l\,L}{0\ 0\ 0}\binom{l`\ l\,L}{0\ 0\ 0}\sum_{j=|j-j`|}^{j+j`}(-1)^j\,(2j+}$$
$$\boldsymbol{1)W(ll`ll`;jL)M_{ll`}^{jm_j}M_{ll`}^{jm`_j}} \qquad (8)$$

And the M –matrix is

$$\boldsymbol{M_{ll`}^{jm_j} = \sum_{mm`hh`p\mu} b_{lhm}^{p\mu}\begin{pmatrix} l\ l`\ j \\ -m\ m`\ m_j \end{pmatrix} b`_{l`h`m`}^{p\mu} T_{lh,l'h`}^{p\mu}}$$
$$(9)$$

From this relationship, it becomes evident that transitions become forbidden when K – K` ≠ m` - m. For spherical top

molecules, the expression for the $\frac{d\sigma}{d\Omega}$ A_L coefficients are determined as follows:

$$\frac{d\sigma}{d\Omega}(J \to J') = \frac{k'}{k} \sum_L A_L (J \to J') P_L(\cos\theta) \qquad (10)$$

$$A_L(j \to j`) = \frac{(2j`+1)(2L+1)(-1)^L}{4k^2(2j+1)} \sum_{ll`\bar{l}l`} j^{l-l`}(-i)^{l-l`}[(2l+1)(2l`+1)(2\bar{l}+1)(2\bar{l}`+1)] \times$$

$$\begin{pmatrix} l & \bar{l} & L \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} l` & \bar{l}` & L \\ 0 & 0 & 0 \end{pmatrix} \sum_{j=|j-j`|}^{j=j`} (-1)^j W(l\bar{l}l`\bar{l}`; jL) M_{l\bar{l}}^{jm_j} M_{l`\bar{l}`}^{jm_j} \quad (11)$$

And the M coefficients take up the same form as that given before for symmetric top molecules.

The first K-matrix elements from the Born series.

To calculate the K-matrix elements for a nonlinear polyatomic molecule, we use the FBA (First Born Approximation) expressions, which are applicable for scattering from a neutral molecular target. These expressions are given as follows:

$$K_{lh,l`h`}^{p\mu} = -2k \int_0^\infty j_l(kr) j_{l`}(kr) r^2 dr \langle X_{lh}^{p\mu} | \sum_{\lambda H} v_\lambda H(r) X_{\lambda H}^{A_l} | X_{l`h`}^{p\mu} \rangle \qquad (12)$$

For the C$_{2v}$ point group

$$\sum_{\lambda H} v_\lambda H(r) X_{\lambda H}^{A_l} = \frac{A}{r^2} S_1^{01} + \frac{B}{r^3} S_2^{01} + \frac{B`}{r^3} S_2^{21} + \frac{C}{r^4} + \cdots \qquad (13)$$

And for the C_{3v} point group

$$\sum_{\lambda H} v_\lambda H(r) X_{\lambda H}^{A_l} = \frac{A}{r^2} S_1^{01} + \frac{B}{r^3} S_2^{01} + \frac{B`}{r^3} S_2^{21} + \frac{C}{r^4} + \frac{C`}{r^4} S_3^{3-1} \cdots \qquad (14)$$

The coefficients A, B, C, and C', on the other hand, are associated with the various moment tensors, including the dipole moment (D), quadrupole moments Q_2^0, Q_2^2 and octupole moments Ω_3^0, Ω_3^3. This relationship is explained with reference to the angular coefficients X's and S's, which are defined in Ref.[17].

$$A = -\left(\frac{4\pi}{3}\right)^{1/2} D. \qquad (15a)$$

$$B = -(4\pi/5)^{\frac{1}{2}} Q_2^0 \qquad (15b)$$

$$B` = -(4\pi/15)^{\frac{1}{2}} Q_2^2 \qquad (15c)$$

$$C = -(4\pi/7)^{\frac{1}{2}} \Omega_3^0 \qquad (15d)$$

$$C` = -(48\pi/35)^{\frac{1}{2}} \Omega_3^3 \qquad (15 e)$$

For the dipole moment $\lambda = H = 1, v_{ll} = -D/r^2$ and $X_{ll}^{A_l} = \left(\frac{4\pi}{3}\right)^{1/2} S_1^{01}$ is obtained by applying Eq (10) After the angular integration.

$$K_{lh,l`h`}^{p\mu} = \frac{2D}{3} \sqrt{(2l+1)(2l`+1) \frac{\sin[(l-l`)\pi/2]}{l(l+1)-l`(l`+1)}} (-1)^m c(ll`1; 000) C(ll`1; m - m_o) \qquad (16)$$

The above K- matrix elements are energy independent.

For the quadruple moment.

$$K_{lh,l`h`}^{p\mu} = -\frac{\pi k}{4} \frac{\Gamma(s-2)(B I_2^{01} + B` I_2^{21})}{\Gamma(s)\Gamma(s-1-\frac{1}{2})(s-l`-\frac{1}{2})} \qquad (17)$$

Where s=1/2(l+l`+1) +1/2 and

$$I_L^{MQ} = \int S_l^{mq} S_L^{MQ} S_{l`}^{m`q`} dr. \qquad (18)$$

III.   RESULTS AND DISCUSSION

While the primary focus of this study is to exploring into the rotational excitation cross sections of polyatomic molecules, we have also conducted calculations for elastic (rotationally resolved) cross sections. These cross sections were derived by iteratively incorporating the rotationally resolved differential cross sections (DCS). The resulting outcomes are depicted for electron scattering DCS with distinct formulations for CH$_4$ molecule, at incident energies of 5, 7.5 and 10 eV. In figure (1) We compared our results of DCS at 5 eV with the theoretical data for the rotational excitation transition from (0-0), (0-3) and (0-4). With Machadoet et al[1] ,Brescansin et al[18]. and Jain et al [19]. And the Expermantail data of Muller etal.[20].
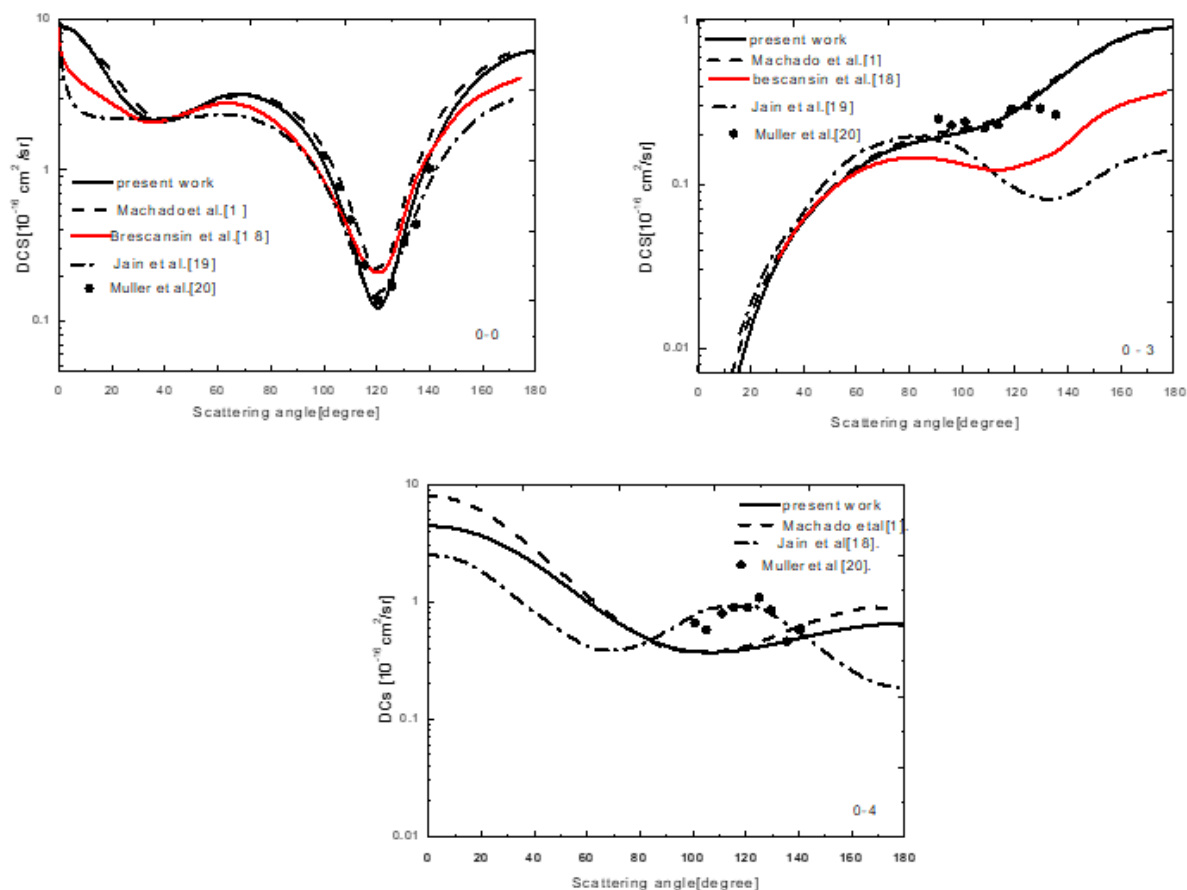
Fig.1:Rotational excitation (J →J`) DCS for the e- CH_4 scattering at 5eV. The full curves are the present results. Other theoretical calculations are due to Machado[1].Brescansin[18] .jain [19].And experimental Muller[20] ,

In figure(2) we compared our results of DCs at 7.5 eV for (0 -0) transition with the theoretical data of Machadoet et al[1] ,Brescansin et al[18]. and Jain et al [19]. and the experimental data with Muller etal.[20], and for the transitions (0-3) ,(0 -4)we compare our data with Machadoet et al[1] ,Brescansin et al[18]. expermantail data of Muller etal.[20].
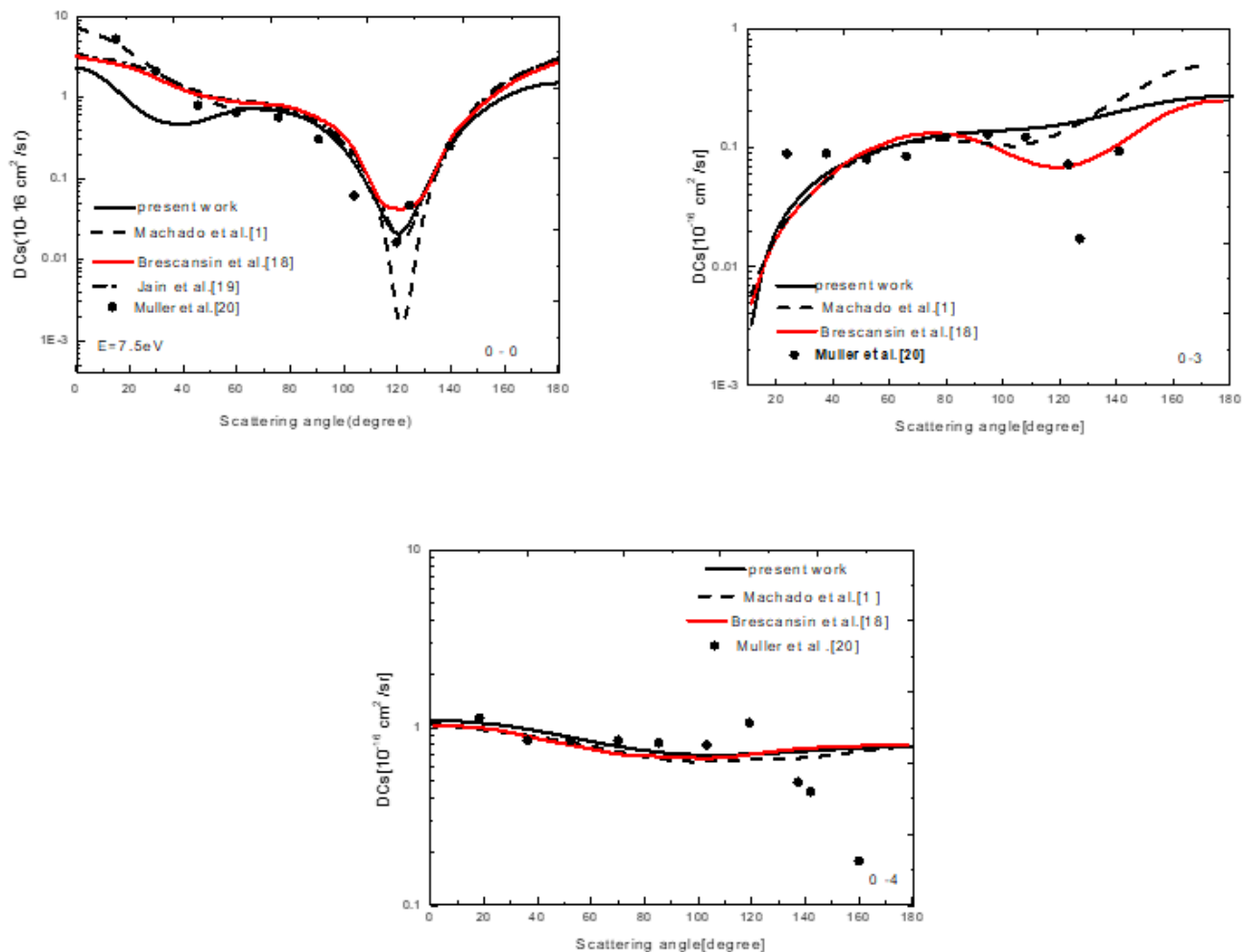
Fig.2: Rotational excitation (J →J`) DCS for the   e- CH_4 scattering at 7.5 [eV]. The full curves are the present results.Other theoretical calculations are due toMachado[1].Brescansin[18] .jain [19].And experimental Muller[20] .

In figure(3)we compared our results of DCS at 10 eV with the theoretical data for   transition   (0-0),(0 -3) and (0 -4)   with   the calculations of   of Machadoet et al[1],Abusalbi et al.[21].and Varella et al.[22].,and the expermantail data of Muller etal.[20]. Finally Figure(4) shows the total cross sections of   transitions (0-0) ,(0-3) and (0-4) compared with the theoretical results of Varella et al.[22].
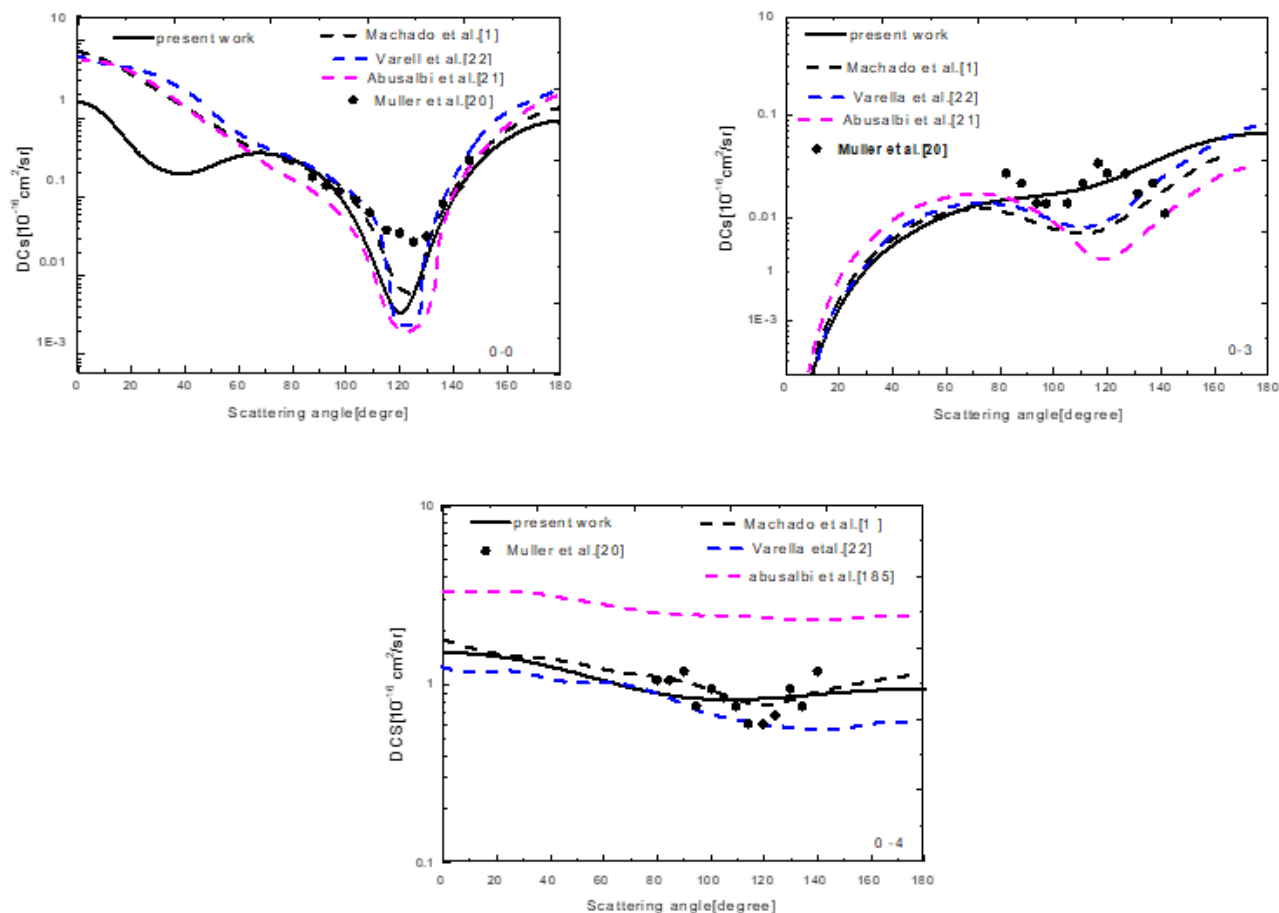
Fig.3: Rotational excitation (J →J`) DCS for the e- CH₄ scattering at 10 eV. The full curves are the present results.Other theoretical calculations are due to Machado[1].Varella[22].Abusalbi [21]. And experimental Muller[20].

In figure(4)we compared our results the total cross sections related to the rotational excitation of the methane molecule, elucidating the transitions in conjunction with a theoretical analysis provided by researcher Varella et al.[10].

In summary, our findings from this study reveal a significant level of agreement between our theoretical and practical results, especially at the energy of 5eV. as depicted in the figure. However, when considering the transition from 0 to 3, we observe a deviation from the findings of researcher Brescansin etal[18]. . This deviation can be attributed to variances in the mathematical methodologies employed. Conversely, in the case of the transition from 0 to 4, our results exhibit strong congruence with those of Machado[7]. Furthermore, at a power of 7.5, our work aligns well with the theoretical and practical outcomes of previous researchers. At an energy of 10, our results correspond with those of researcher Machado[7] , while deviations from other researchers' findings can be ascribed to differences in computational methods employed.

IV.   CONCLUSION

This study focuses on a theoretical analysis of low-energy electron scattering by polyatomic CH_4 molecules. We provide rotationally elastic and inelastic cross-sectional data, as well as rotationally cross sections, which we compare to existing experimental and theoretical findings. Our calculated rotationally cross sections generally exhibit strong agreement with measured data that lacks rotational resolution. This robust consistency lends support to the interaction dynamics described in our study and the methodologies employed for solving the scattering equations. Furthermore, we are actively working on extending this analysis to encompass higher incident energies and different molecular targets.

The findings indicate that, in comparison to other researchers who employed the adiabatic nuclei rotation approximation method, the Boar method demonstrated favorable agreement for transitions 0-0 and 0-3.
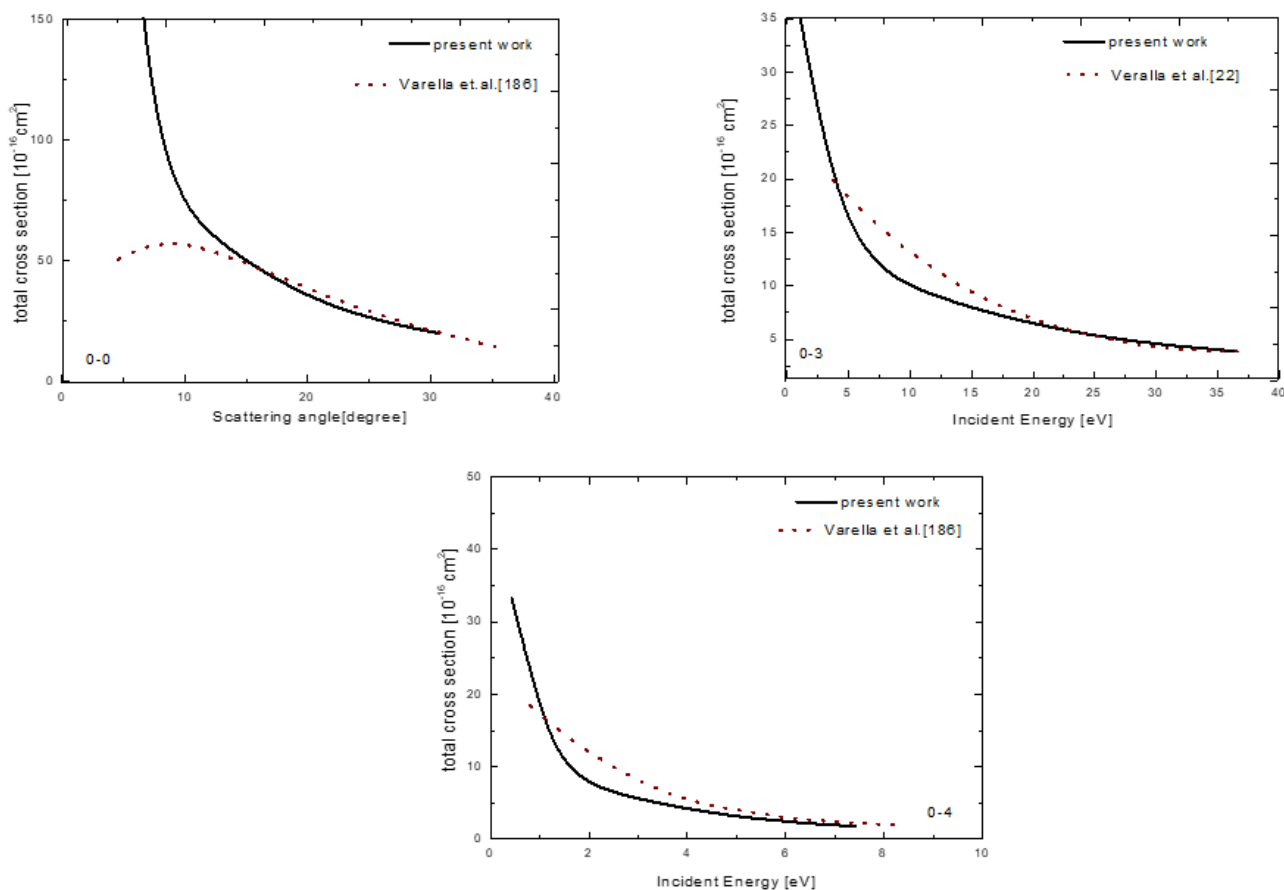
Fig.4: The diagram illustrates the total cross sections related to the rotational excitation of the methane molecule, elucidating the transitions in conjunction with a theoretical analysis provided by researcher Varella et al.[10].

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