



Investigation of Electron Scattering from Vinyl Ether and Its Isomers

Himani Tomer ¹, Biplab Goswami ² and Bobby Antony ¹,*

- ¹ Department of Physics, Indian Institute of Technology (Indian School of Mines), Atomic and Molecular Physics Laboratory, Dhanbad 826004, India; himanitomer22@gmail.com
- ² Gaya College of Engineering, Srikrishna Nagar, Khizarsarai 823003, India; biplab.goswami10@gmail.com
- Correspondence: bobby@iitism.ac.in

Abstract: This article reports a comprehensive theoretical study of electron scattering from vinyl ether and its isomers. The electron-molecule quantum collision problem is solved through a complex optical potential approach. From the solution of the Schrödinger equation corresponding to this scattering problem, various cross sections were obtained for energies from ionization threshold of target to 5 keV. To deal with the non-spherical and complex structure, a multi-center group additivity approach is used. Furthermore, geometrical screening correction is applied to compensate for the overestimation of results due to electron charge density overlap. We found an interesting correlation between maximum ionization cross section with polarizability and ionization energy of the target molecule. The fitting of the total cross section as a function of the incident electron energy is reported in this article. The correlation between the effective diameter of the target and the projectile wavelength at maximum ionization energy is also reported for vinyl ether and its isomers. The data presented here will be useful to biomedical field, mass spectrometry, and chemical database for military range applications. The cross sections are also important to model Mars's atmosphere due to their presence in its atmosphere. The gas-kinetic radius and the van der Waals coefficients are estimated from the electron-impact total scattering cross sections. In addition, the current study predicts the presence of isomeric effects in the cross section.

Keywords: electron scattering; elastic cross section; inelastic cross section; vinyl ether; isomeric effect; optical potential method

1. Introduction

The molecule with the formula C_4H_6O has six structural isomers: vinyl ether, 2-butenal, cis-2-butenal, cyclobutanone, furan, 2, 3-dihydro, and furan, 2, 5-dihydro. Vinyl ether is an important molecule for biomedical applications. It is used as an anesthetic in surgical procedures in children for short durations with fast recovery time [1]. Mass spectrometry is one of the techniques to monitor gas concentration for the patient undergoing an anaesthetic procedure [2]. Vinyl ether is also used as an antioxidant to reduce the side effect of free radicals (oxidants) in the human body that can cause genetic disorders [3,4]. There is a possibility of having free electrons and oxidants (having unpaired electrons in the outermost shell) in the human body for further reaction to damage DNA [3,4]. Plasmalogens (endogenous antioxidants) containing vinyl ether bonds are found in high concentrations in brain and heart [5]. Plasmalogens deficiency can cause neurodegenerative diseases, cancer, stroke, etc. [6,7]. Hence, to understand the chemistry of this biological environment, one needs to model the system with various cross sections and reaction rates as input. Another important application of C_4H_6O molecule is in the military, where it is considered as a range compound [8], and its cross section and rate coefficients are useful in gas transport modeling. The presence of C_4H_6O on the surface of Martian soil was detected as early as 1977 [9]. Natural processes make it possible to create this molecule in the atmosphere of



Citation: Tomer, H.; Goswami, B.; Antony, B. Investigation of Electron Scattering from Vinyl Ether and Its Isomers. *Atoms* **2022**, *10*, 43. https:// doi.org/10.3390/atoms10020043

Academic Editor: Grzegorz Piotr Karwasz

Received: 23 March 2022 Accepted: 22 April 2022 Published: 24 April 2022

Publisher's Note: MDPI stays neutral with regard to jurisdictional claims in published maps and institutional affiliations.



Copyright: © 2022 by the authors. Licensee MDPI, Basel, Switzerland. This article is an open access article distributed under the terms and conditions of the Creative Commons Attribution (CC BY) license (https:// creativecommons.org/licenses/by/ 4.0/). Mars [10]. Furan, 2, 5-dihydro is used in pharmaceuticals and commodity chemicals [11] as well.

The wide range of applications for C_4H_6O molecule from biological sciences to atmospheric physics has encouraged us to perform the present calculations. To the best of our knowledge, there is no previous data available to compare our results in the energy range chosen here (from ionization potential of the target molecule to 5 keV). The only single data point available is from Tureček et al. [12], who evaluated relative ionization cross section value for cis-2-butenal, cyclobutanone, and furan, 2, 5-dihydro at 75 eV. Due to the unavailability of previously reported data, our results are compared with another molecule with similar structure, i.e., tetrahydrofuran (THF). THF and furan, 2, 5-dihydro have a similar structure "(with THF having 2 additional electrons)" and very close ionization energy and electric dipole polarizability, thus making it a good candidate for comparison. Theoretical and experimental data for THF are available in the literature [13–19].

The present study of electron scattering from C₄H₆O and its isomers has been performed based on spherical complex optical potential formalism (SCOP) [20,21] and complex scattering potential ionization contribution method (CSP-ic) [20,21]. The theoretical approach of SCOP evaluates integral elastic (Q_{el}) and inelastic (Q_{inel}) cross section values. The addition of these two cross sections provides the total (Q_{tot}). The CSP-ic method is applied to evaluate ionization cross section (Q_{ion}). The electrostatic potential surface method is employed to identify the centers that scatters the incoming electron. Due to the non-spherical and complex structure of these targets, a multi-center approach called group additivity rule is used [22], which could predict reasonable cross sections. Further fine tuning is performed by a geometrical screening correction technique to compensate for the overestimation in cross section due to overlapping of electron charge densities. The Q_{el} , Q_{ion} , and Q_{tot} values for vinyl ether and its isomers are reported first. The correlation of Q_{ion}^{max} with (α/I)^{1/2} and effective target diameter (d_{rms}) and the projectile wavelength (λ_{max}) for vinyl ether and its isomers produces a good understanding of ionization cross section and molecular parameters.

Furthermore, a parametric fitting of $Q_{tot}(E_i)$ with energy $(A(E_i)^{-B})$ at the intermediate energy range shown. Present electron-impact total scattering cross sections are then utilized to estimate the gas-kinetic radius and van der Waals coefficients. The theoretical description is given in Section 2, and Section 3 explains the present results. The final section concludes with an overall summary of the work.

2. Theoretical Methodology

Present target molecules, C_4H_6O and its isomers, are structurally complex and large in size in terms of an electron-molecule quantum collision problem. The geometries of the present target molecules are shown in Figure 1, while in Table 1, their ionization energies and polarizabilities are illustrated. Due to this reason, a target molecule is divided into groups/scattering centres to have a viable calculation and to obtain reasonable cross-section values. These scattering centers are identified based on molecular geometrical configuration and its electron charge density distribution. For the present set of molecules, these centers are identified through Avogadro software [23] using the electrostatic potential surface method, as shown in Figure 2.

Table 1. The ionization energy (*I*) and polarizability (α) of the targets [24].

Target	<i>I</i> (eV)	α (Å ³)
Vinyl Ether	8.680	7.841
2-butenal	9.750	8.50
Cis-2-butenal	9.750	7.762
Cyclobutanone	9.354	6.940
Furan, 2, 3-dihydro	8.837	6.951
Furan, 2, 5-dihydro	9.160	7.058



Figure 1. The structure of the targets: (1) vinyl ether, (2) 2-butenal, (3) cis-2-butenal, (4) cyclobutanone, (5) furan, 2, 3-dihydro, and (6) furan, 2, 5-dihydro.



Figure 2. Scattering centres identified using Avogadro software by electrostatic potential surface method: (1) vinyl ether, (2) 2-butenal, (3) cis-2-butenal, (4) cyclobutanone, (5) furan, 2, 3-dihydro, and (6) furan, 2, 5-dihydro.

For each scattering center, total charge density is calculated via expansion of charge density of individual atoms from the center of mass of that particular group. In the present case, the scattering center contains more than one heavier atom along with hydrogen atoms. The expansion of charge density for heavier atoms is performed from the center of mass, and for hydrogen atoms, charge density expansion is induced by heavier atoms. This expanded charge density is re-normalized to obtain the total number of electrons in each scattering centre. The charge density $\rho(r)$ is calculated using the atomic parameters as described in Cox and Bonham [25]. For each scattering centre, the Schrödinger equation comprises complex optical potential and solves it with the help of partial wave method. This method is called the group additivity rule (GAR) [22]. From the contribution of each

scattering center, the overall cross section of the target molecule is calculated. Further information on this methodology may be obtained from the articles [26,27].

The potential includes all standard possible projectile-target interactions. The optical potential (V_{opt}) consists of real (V_R) and imaginary (V_I) parts expressed as follows.

$$V_{opt}(r, E_i) = V_R(r, E_i) + i V_I(r, E_i).$$
 (1)

Here, E_i is the projectile field energy in eV and r is the projectile-target interaction distance. V_R comprises static potential (V_{st}), exchange potential (V_{ex}), and polarization potential (V_{pol}) modeled from [25,28,29], respectively. V_{st} is experienced by the incoming electron due to target's static charge cloud. V_{ex} occurs due to the interaction and the exchange of incident and target electrons. V_{pol} arises via the redistribution of target charge cloud by the interaction with incident field, which creates a perturbation in static charge cloud. V_I in Equation (1) corresponds to the absorption of incident flux due to inelastic channels such as excitation and ionization, which is modeled using the non-empirical formula reported by Staszewska et al. [30,31]. The solution of Schrödinger equation is obtained as phase shifts (δ_I), possessing the signature of all scattering channels. Using these complex phase shifts, the cross sections are estimated as follows [20,21]:

$$Q_{el}(E_i) = \frac{\pi}{k^2} \sum_{l=0}^{\infty} (2l+1) |\eta_l \exp(2iRe\,\delta_l) - 1|^2,$$
(2)

$$Q_{inel}(E_i) = \frac{\pi}{k^2} \sum_{l=0}^{\infty} (2l+1)(1-\eta_l^2),$$
(3)

where *k* is the wave vector, and $\eta_l = \exp(-2Im\delta_l)$ is the 'inelasticity' or 'absorption factor' for each partial wave *l*. The sum of elastic and inelastic cross section provides the total cross section. Furthermore, ionization cross section is estimated through an energy-dependent ratio, *R*(*E*_{*i*}) based on CSP-ic method [20,21]. The ratio is defined as follows:

$$R(E_i) = \frac{Q_{ion}(E_i)}{Q_{inel}(E_i)},\tag{4}$$

such that $0 < R \le 1$ following the boundary conditions:

$$R(E_i) \begin{cases} = 0, \text{ for } E_i \leq I \\ = R_p, \text{ at } E_i = E_p \\ \cong 1, \text{ for } E_i >> E_p \end{cases}$$
(5)

where E_P is the energy where Q_{inel} reaches its maximum value. The first choice in Equation (5) confirms that the target's ionization channel is not active below its threshold *I*. The second condition represents the contribution of ionization in the inelastic cross section is R_P (about 70–80%) [32] at peak energy (E_P). This is an empirical estimation based on benchmark experimental/theoretical results. According to the third condition, $R(E_i)$ approaches unity as projectile energy increases. In the present calculations, we have taken $R_P = 0.70$ for all targets. Using this $R(E_i)$, Q_{ion} is predicted with an uncertainity of approximately $\pm 7\%$, which is termed as the CSP-ic method [20,21].

For all these molecules, a screening correction technique is applied [33] to obtain reliable cross sections. As the number of atoms in a molecule increases, the possibility of screening effect due to charge density overlapping of atoms within the molecule also enhances. This overlapping causes an overestimation of cross section from its actual values. Hence, a geometrical screening correction technique is applied for the present target molecules to overcome this. The present calculation considers a screening correction to the central atom of an individual group. The screening correction between the groups is not considered as the charge overlapping between the groups is assumed to be negligible. The screening correction included in the present calculation is explained below. The overlap cross section for each group is calculated with the following.

$$Q_{OL}(group) = \frac{1}{N} \sum \frac{Q_i Q_j}{\alpha_{ij}}.$$
(6)

Here, *N* provides the number of neighboring atoms of the central atom. Q_i and Q_j represent the cross section values of *i*th and *j*th atoms of these neighbors. α_{ij} is the max $(4\pi r_{ij}^2, Q_i, Q_j)$ and r_{ij} the distance between *i*th and *j*th atoms. Thus, the screening corrected cross section Q_{SC} for the scattering group is obtained as follows:

$$Q_{SC} = Q_{GAR} - Q_{OL},\tag{7}$$

where Q_{GAR} is the cross section calculated based on the group additivity rule.

3. Results and Discussion

This section presents the cross sections predicted for all the targets studied. The cross section is plotted along y-axis in Å² and energy along x-axis in eV (logarithmic scale). The present results are compared with THF, both theoretical [13,14] and experimental [16–19] cross sections, due to the non-availability of previous data for vinyl ether and its isomers. The structure of THF and furan, 2, 5-dihydro is quite similar, except for the difference of two hydrogen atoms. In addition, the target parameters such as the ionization threshold and polarizabilities are also close to each other, which makes the comparison justified.

In Figure 3, present furan, 2, 5-dihydro cross section values are presented and compared with previous data of THF computed by Swadia et al. [13], Fuss et al. [18], and Mozejko et al. [14] and measured by Baek et al. [19]. The theoretical values by Swadia et al. [13] are comparable in the 18–30 eV energy range, but they are higher beyond that. Swadia et al. [13] obtained Q_{el} through the optical potential approach and, hence, is similar to the present calculation. The values of Fuss et al. [18] are lower than the present result up to 50 eV, while their results are comparable above that. At higher energies, both results merge together. Fuss et al. [18] computed Q_{el} by using a screening-corrected independent atom approach using the optical potential. The difference in additivity rule and screening correction method used in present and Fuss calculations creates the deviation in the outputs. Mozejko et al. [14] results are higher than present outcomes throughout the energy range. The method employed by Mozejko is different than the present approach. In addition, they have used an independent atom model (IAM) approach, which does not consider the redistribution of atomic electrons due to molecular bonding and, hence, produces higher values compared to the present result. However, above 400 eV, they are comparable to each other as the projectile electron obtains less time to spend with the target. The experimental data of Baek et al. [20] are quite close to the present values throughout the energy range within the experimental error.

In Figure 4, present Q_{tot} results are presented along with comparison (THF) [13,17–19]. The values for THF are in general lower than our cross section below 50–80 eV. Beyond that, the total cross section agrees quite well with all the available data for THF. The theoretical curves of Fuss et al. [18] are much lower than all others up to about 200 eV. However, the measurements of Fuss et al. [18] produce an excellent agreement with present results throughout the energy range. The experimental result of Mozejko et al. [17] is lower than present curve around the ionization threshold region and then become comparable above 60–80 eV. The same is true for the measurements of Baek et al. [19] as well.



Figure 3. Q_{el} for furan, 2, 5-dihydro. Solid line: present Q_{el} ; dash line: Q_{el} for THF by Swadia et al. [13]; dotted line: Q_{el} for THF by Fuss et al. [18]; dash-dot line: Q_{el} for THF by Moze-jko et al. [14]; solid circle: Q_{el} for THF by Baek et al. [19].



Figure 4. Q_{tot} for furan, 2, 5-dihydro. Solid line: present Q_{tot} ; dash line: Q_{tot} for THF by Swadia et al. [13]; dotted line: Q_{tot} for THF by Fuss et al. [18]; solid triangle: Q_{tot} for THF by Fuss et al. [18]; solid star: Q_{tot} for THF by Mozejko et al. [17]; solid circle: Q_{tot} for THF by Baek et al. [19].

Figures 5–7 show present ionization cross section values of furan, 2, 5-dihydro, cis-2butenal, and cyclobutanone, respectively. In Figure 5, the present Q_{ion} of furan, 2, 5-dihydro compares with the experimental and theoretical data points of furan, 2, 5-dihydro from Tureček et al. [12]. Present Q_{ion} values of furan, 2, 5-dihydro are also compared with THF values reported by Swadia et al. [13] and Mozejko et al. [14] and the experimental values given by Fuss et al. [18] and Dampc et al. [16]. Present values are higher than all other data near the intermediate energy range. However, it merges with most of them at low and high energies. Mozejko et al. [14] computed Q_{ion} using the Binary-Encounter-Bethe (BEB) model, which estimates direct ionization cross-sections for the ground states of the geometrically optimized molecule. Present Q_{ion} values are comparable to the experimental result of Fuss et al. [18] within their error bars. Moreover, it shows excellent agreement with the measurements of Dampc et al. [16] up to 30 eV. The experimental data points of Tureček et al. [12] is significantly less than the present values at 75 eV, while the theoretical data point is slightly close to present data and much closer to that of THF values. In Figure 6, the theoretical and experimental data points of Tureček et al. [12] is compared with the present data for cis-2-butenal. The data points at 75 eV are quite lower than our results. In Figure 7, the cross section for cyclobutanone is plotted along with the data point at 75 eV by Tureček et al. [12]. This is similar to the previous figure, except that they do not agree with each other.



Figure 5. Q_{ion} for furan, 2, 5-dihydro. Solid line: present Q_{ion} ; dash line: Q_{ion} for THF by Swadia et al. [13]; dotted line: Q_{ion} for THF by Mozejko et al. [14]; solid triangle: Q_{ion} for THF by Fuss et al. [18]; solid circle: Q_{ion} for THF by Dampc et al. [16]; solid rhombus and solid hexagonal: experimental Q_{ion} for furan, 2, 5-dihydro by Tureček et al. [12] and solid star: theoretical Q_{ion} for furan, 2, 5-dihydro by Tureček et al. [12].



Figure 6. Q_{ion} for cis-2-butenal. Solid line: present Q_{ion} for cis-2-butenal; solid rhombus: theoretical Q_{ion} calculated for cis-2-butenal by Tureček et al. [12]; solid hexagonal: experimental Q_{ion} calculated for cis-2-butenal by Tureček et al. [12].



Figure 7. Q_{ion} for cyclobutanone. Solid line: present Q_{ion} for cyclobutanone; solid rhombus: theoretical Q_{ion} calculated for cyclobutanone by Tureček et al. [12]; solid hexagonal: experimental Q_{ion} calculated for cyclobutanone by Tureček et al. [12].

Figures 8 and 9 represent Q_{el} and Q_{tot} for vinyl ether and its isomers, respectively. Near the ionization threshold, the difference in cross sections of isomers is enough to visualize the isomeric effect in the present target molecules. This difference decreases at the intermediate energy range, and at higher energies cross section values are close to each other. The isomeric effect is due to the difference in the structure of isomers and, hence, the distribution of charge density of individual atoms in the target molecule. C_4H_6O have branched and cyclic structures, which is contributing to the isomeric effect. Vinyl ether, 2-butenal, and cis-2-butenal are branched isomers. The Q_{el} and Q_{tot} values of 2-butenal and cis-2-butenal are quite close throughout the energy range except between 10-14 eV. The hump at low energy in Q_{tot} is enhanced due to the inclusion (or opening) of more inelastic channels while calculating elastic cross sections. In contrast, the cross section for vinyl ether is different from 2-butenal and cis-2-butenal, reflecting the electron cloud and polarizability of the branched isomers. The cyclic isomers, furan, 2, 3-dihydro, and furan, 2, 5-dihydro have similar Q_{el} and Q_{tot} values throughout the energy range except for the 10–17 eV and 15–30 eV energy ranges, respectively. Cyclobutanone, another cyclic isomer, has different Q_{el} and Q_{tot} values than furan, 2, 3-dihydro and furan, 2, 5-dihydro near-ionization threshold, and intermediate energy range, which shows structural effect. However, at high energies, the isomeric effect vanishes for all targets. This is because, as the incident electron field energy increases, the de Broglie wavelength of the incident electron becomes so small that it does not recognize molecular structures any more. Thus, the structural effects and/or threshold effects become negligible, and the isomeric effect in cross section disappears.



Figure 8. Q_{el} for vinyl ether and its isomers. Solid line: present Q_{el} for vinyl ether; dash line: present Q_{el} for 2-butenal; dotted line: present Q_{el} for cis-2-butenal; dash-dot line: present Q_{el} for cyclobutanone; dash-dot-dot line: present Q_{el} for furan, 2, 3-dihydro; short dash line: present Q_{el} for furan, 2, 5-dihydro.



Figure 9. Q_{tot} for vinyl ether and its isomers. Solid line: present Q_{tot} for vinyl ether; dash line: present Q_{tot} for 2-butenal; dotted line: present Q_{tot} for cis-2-butenal; dash-dot line: present Q_{tot} for cyclobutanone; dash-dot-dot line: present Q_{tot} for furan, 2, 3-dihydro; short dash line: present Q_{tot} for furan, 2, 5-dihydro.

To study the consistency and reliability of the data, we have also analytically fitted the total cross section at intermediate and high energy range (100–1000 eV) using the following formulae [34]:

$$Q_{tot}(E_i) = A(E_i)^{-B},\tag{8}$$

where A and B are fitting parameters and E_i is the incident electron energy. The fitting given by Joshipura et al. [34] is for the molecular systems having 10 electrons. Furthermore, Garcia et al. [35] has also reported such fittings of the total cross section at intermediate energies for molecules having 10–22 electrons. The resent target molecules and its isomers

have 38 electrons. The calculated and fitted cross sections are given in Figure 10. It shows excellent corroboration and proves the validity of our data. The parameters A and B are given in Table 2. We can see that the value of B is quite close for all the isomers, while parameter A varies quite significantly. Since the magnitude of total cross section can be considered as a size-effect, it should depend on the spread of an electron cloud, which is reflected by the polarizability of the molecule.



Figure 10. The correlation plot of $Q_{tot}(E_i)$ with $A(E_i)^{-B}$ for vinyl ether and its isomers. Solid star: present Q_{tot} data points; solid line: analytical fitting function $A(E_i)^{-B}$.

Table 2. The fitting parameters of Equation (8). Gas-kinetic radius (R_g) and van der Waals coefficient (*b*) of the present molecules.

Target	Α	В	R_g (Å)	b (L mol ^{-1})
Vinyl Ether	780.545	0.681	2.181	0.1047
2-butenal	677.087	0.662	2.146	0.0998
Cis-2-butenal	675.835	0.662	2.144	0.0995
Cyclobutanone	687.329	0.663	2.158	0.1015
Furan, 2, 3-dihydro	709.75	0.662	2.206	0.1083
Furan, 2, 5-dihydro	711.352	0.665	2.189	0.1058

Furthermore, the gas-kinetic radius (R_g) and van der Waals coefficient (b) are two important quantities for characterizing the motion of any molecules in the gas phase. A formula for calculation the gas-kinetic radius (R_g) and the van der Waals coefficient (b) using total electron scattering cross-sections (TCS) was given in Hirschfelder et al. [36].

$$R_g = \sqrt{\frac{Q_{tot}}{\pi}} \tag{9}$$

and the following is the case.

$$b = 4N_A \frac{4}{3}\pi R_g^{3}.$$
 (10)

Here, N_A is the Avogadro number. The R_g and b calculated for the present targets are listed in Table 2. It can be observed that only minor variations are seen in R_g and b due to the same electron number, which is slightly different due to change in geometrical distribution of the constituent atoms. For the present isomers, the maximum change in position of the center of mass is only about 9% by the rearrangement of C, H and O atoms in these molecules. A similar effect is observed in the previous calculations of Goswami et al. [38].

In Figure 11, the total ionization cross sections for vinyl ether and its isomers were compared. The graph shows that the cross section values for vinyl ether are more prominent in magnitude than other isomers. The curves of furan, 2, 3-dihydro and furan, 2, 5-dihydro are very close throughout the energy range. In contrast, the values of 2-butenal and cis-2-butenal cross sections merges together. The cross section for cyclobutanone is very close to furan, 2, 5-dihydro below 40 eV. The peak of present ionization cross section is at 60 eV for vinyl ether, cyclobutanone, furan, 2, 3-dihydro, and furan, 2, 5-dihydro and at 70 eV for 2-butenal and cis-2-butenal.



Figure 11. Q_{ion} for vinyl ether and its isomers. Solid line: present Q_{ion} for vinyl ether; dash line: present Q_{ion} for 2-butenal; dotted line: present Q_{ion} for cis-2-butenal; dash-dot line: present Q_{ion} for cyclobutanone; dash-dot-dot line: present Q_{ion} for furan, 2, 3-dihydro; short dash line: present Q_{ion} for furan, 2, 5-dihydro.

For a particular incident energy, the wavelength of the projectile electron matches molecular diameter and gives maximum cross section values. Harland et al. [39] showed that the effective diameter of the molecule may be obtained using the radius of the polarizability sphere. The radius of the polarizability sphere is obtained through the polarizability volume of the target molecule. The present target molecule has six different structural formulas with 38 electrons. The electron cloud of a molecule is proportional to its polarizability volume. The polarizability volume provides an idea of molecular charge distribution and adequate sizes of the molecule. Figure 12 represents the relation between effective molecular diameter, d_{rms} and incident electron wavelength at Q_{ion}^{max} . In Figure 12, the effective diameter of each isomer is slightly higher than the electron wavelength at which Q_{ion} attains its maximum value. The incident electron at the de Broglie wavelength of 1.462 Å and 1.579 Å is comparable to the effective diameter of 2-butenal and cis-2-butenal and vinyl ether, cyclobutanone, furan, 2, 3-dihydro, and furan, 2, 5-dihydro, respectively. The probability of ionization increases from the threshold region and reaches its maximum value as the de Broglie wavelength of incident electron matches to an effective diameter of the target molecule.



Figure 12. The correlation between the effective molecular diameter, d_{rms} , and the incident electron wavelength, λ_{max} , at a maximum of ionization cross section for vinyl ether and its isomers. (1): vinyl ether; (2): 2-butenal; (3): cis-2-butenal; (4): cyclobutanone; (5): furan, 2, 3-dihydro; (6): furan, 2, 5-dihydro.

The maximum ionization cross section value also depicts the relation between polarizability and ionization energy of the target molecule. Figure 13 represents the relationship of Q_{ion}^{max} with $(\alpha/I)^{\frac{1}{2}}$ for vinyl ether and its isomers. In Figure 13, the correlation of Q_{ion}^{max} with $(\alpha/I)^{\frac{1}{2}}$ for vinyl ether, cyclobutanone, furan, 2, 3-dihydro, and furan, 2, 5-dihydro is close to a straight line. On the other hand, for 2-butenal and cis-2-butenal, the correlation is quite small. The polarizability value for 2-butenal is slightly higher than cis-2-butenal, making the point falls towards the right in the figure. The reliability of the present Q_{ion}^{max} is also estimated through the relation $Q_{ion}^{max} = 11.92 (\alpha/I)^{\frac{1}{2}}$, as given in Harland et al. [39] and is shown in Table 3.

Table 3. Comparison of present maximum ionization cross section value with the relation given in Harland et al. [39].

Target	Present Q _{ion} ^{max}	$Q_{ion}^{max} = 11.92 (\alpha/I)^{\frac{1}{2}}$
Vinyl Ether	16.528	11.324
2-butenal	14.091	11.133
Cis-2-butenal	14.093	10.633
Cyclobutanone	14.682	10.263
Furan, 2, 3-dihydro	15.28	10.573
Furan, 2, 5-dihydro	14.934	10.466



Figure 13. The correlation of Q_{ion}^{max} with $(\alpha/I)^{\frac{1}{2}}$ for vinyl ether and its isomers. (1): vinyl ether, (2): 2-butenal, (3): cis-2-butenal, (4): cyclobutanone, (5): furan, 2, 3-dihydro, (6): furan, 2, 5-dihydro.

4. Conclusions

The present study explores the electron-induced scattering cross sections for vinyl ether and its isomers. The cross-section values are essential for studying biological systems, mass spectrometry, military range chemical database, and modeling Mars's atmosphere. SCOP formalism [20,21] and CSP-ic method [20,21] is applied to obtain total, elastic, inelastic and ionization cross section values. The electrostatic potential surface method and group additivity rule [22] is used to perform calculations for cross sections appropriately. Screening correction [33] included in this work refines the cross section from overestimation due to the overlap of electron charge cloud. This is quite evident from the results at the ionization threshold region. Due to the unavailability of previous data, we have compared our results with THF, as furan, 2, 5-dihydro has very similar structure, *I*, and *a* values to that of THF. The electron charge distribution for furan-2-5-dihydro (C_4H_6O) and THF (C_4H_8O) is very much identical. The present result shows reasonable agreement to the theoretical and experimental reported data [12–19].

It also predicts isomeric effect, which is pronounced near the ionizaiton threshold and intermediate energy region for Q_{el} and Q_{tot} . As the incident field energy increases, interaction time decreases; hence, isomeric effect vanishes. The present calculation for 6 isomers with 38 electrons is an interesting study in terms of electron scattering. Electron distribution in each isomer creates the difference in cross section value, which is an observable near-threshold region. The incident electron with low kinetic energy has enough time to visualize the charge distribution, which can be observed through the outputs. We have also presented an analytical analysis of the $Q_{tot}(E_i)$ through a simple relation, $A(E_i)^{-B}$. The current Q_{tot} values are further employed to calculate the gas-kinetic radius (R_g) and van der Waals coefficient (b) for characterizing the motion of present target molecules in the gas phase and astrophysical plasma modeling applications. The correlation graphs of Q_{ion}^{max} with $(\alpha/I)^{\frac{1}{2}}$, and d_{rms} with λ_{max} are made and studied. The current study improves the understanding of the interaction of adequate molecular size and electron wavelength. Furthermore, it also helps in obtaining a better insight into the probability of increasing and decreasing ionization channels for each isomer. The cross section and correlations studied here enhances the understanding of these isomers.

Author Contributions: H.T.: Conceptualization, data curation, writing—original draft preparation, and investigation. B.G.: Calculations for target parameters, gas-kinetic radius and van der Waals coefficients. B.A.: Conceptualization, methodology, software, and writing—Reviewing and Editing.

Funding: The support of this research by Department of Space, Govt of India through ISRO-RESPOND project Grant No. DS-2B-13012(2)/2/2017.

Acknowledgments: BA is pleased to acknowledge the support of this research by Department of Space, Govt of India, through ISRO-RESPOND project Grant No. DS-2B-13012(2)/2/2017.

Institutional Review Board Statement: Not applicable.

Informed Consent Statement: Not applicable.

Data Availability Statement: Data available upon request from the authors.

All authors have read and agreed to the published version of the manuscript.

Conflicts of Interest: No conflicts of interest. The funders had no role in the design of the study; in the collection, analyses, or interpretation of data; in the writing of the manuscript; or in the decision to publish the results.

References

- Gross, R.E. The Use of Vinyl Ether (Vinethene) in Infancy and Childhood: Report of 100 Cases. N. Engl. J. Med. 1939, 220, 334–336. [CrossRef]
- 2. Duncan, A.; Oliver, W.P. Measurement of gas concentrations. Anaesth. Intensive Care Med. 2021, 22, 190–193. [CrossRef]
- Deng, Y.; Zakaria, A.A. Evolution of cubic membranes as antioxidant defence system. *Interface Focus* 2015, *5*, 20150012. [CrossRef]
 [PubMed]
- 4. D'Agosto, F.; Charreyre, M.T.; Pichot, C.; Mandrand, B. Polymer of controlled chain length carrying hydrophilic galactose moieties for immobilization of DNA probes. *Macromol. Chem. Phys.* **2002**, 203, 146–154. [CrossRef]
- 5. Zoeller, R.A.; Lake, A.C.; Nagan, N.; Gaposchkin, D.P.; Legner, M.A.; Lieberthal, W. Plasmalogens as endogenous antioxidants: Somatic cell mutants reveal the importance of the vinyl ether. *Biochem. J.* **1999**, *338*, 769–776. [CrossRef]
- Mankidy, R.; Ahiahonu, P.W.; Ma, H.; Jayasinghe, D.; Ritchie, S.A.; Khan, M.A.; Su-Myat, K.K.; Wood, P.L.; Goodenowe, D.B. Membrane plasmalogen composition and cellular cholesterol regulation: A structure activity study. *Lipids Health Dis.* 2010, 9, 1–17. [CrossRef]
- Wood, P.L.; Khan, M.A.; Smith, T.; Goodenowe, D.B. Cellular diamine levels in cancer chemoprevention: Modulation by ibuprofen and membrane plasmalogens. *Lipids Health Dis.* 2011, 10, 1–8. [CrossRef] [PubMed]
- Zakikhani, M.; Dortch, M.S.; Gerald, J.A. Compilation of Physical and Chemical Properties and Toxicity Benchmarks for Military Range Compounds. ERDC/EL. 2002; TR-02–27. Available online: https://erdc-library.erdc.dren.mil/jspui/bitstream/11681/70 12/1/EL-TR-02-27.pdf (accessed on 22 March 2022).
- Biemann, K.; Oro, J.; Toulmin, P., III; Orgel, L.E.; Nier, A.O.; Anderson, D.M.; Simmonds, P.G.; Flory, D.; Diaz, A.V.; Rushneck, D.R.; Biller, J.E.; Lafleur, A.L. The search for organic substances and inorganic volatile compounds in the surface of Mars. *J. Geophys. Res.* 1977, 82, 4641–4658. [CrossRef]
- 10. Smith, K.A.; Ball, T.; Conen, F.; Dobbie, K.E.; Massheder, J.; Rey, A. Exchange of greenhouse gases between soil and atmosphere: Interactions of soil physical factors and biological processes. *Eur. J. Soil Sci.* **2018**, *69*, 10–20. [CrossRef]
- Brichacek, M.; Njardarson, J.T. Creative approaches towards the synthesis of 2, 5-dihydro-furans, thiophenes, and pyrroles. One method does not fit all! Org. Biomol. Chem. 2009, 7, 1761–1770. [CrossRef]
- 12. Tureček, F.; Brabec, L.; Hanuš, V.; Zima, V.; Pytela, O. Relative ionization cross-sections of oxygenated C (4) molecules. *Int. J. Mass Spectrom. Ion Process.* **1990**, *97*, 117–124. [CrossRef]
- Swadia, M.; Thakar, Y.; Vinodkumar, M.; Limbachiya, C. Theoretical electron impact total cross sections for tetrahydrofuran (C₄H₈O). *Eur. Phys. J. D* 2017, *71*, 1–5. [CrossRef]
- Możejko, P.; Sanche, L. Cross sections for electron scattering from selected components of DNA and RNA. *Radiat. Phys. Chem.* 2005, 73, 77–84. [CrossRef]
- 15. Champion, C. Quantum-mechanical predictions of electron-induced ionization cross sections of DNA components. *J. Chem. Phys.* **2013**, *138*, 184306. [CrossRef]
- Dampc, M.; Szymańska, E.; Mielewska, B.; Zubek, M. Ionization and ionic fragmentation of tetrahydrofuran molecules by electron collisions. J. Phys. At. Mol. Opt. Phys. 2011, 44, 055206. [CrossRef]
- 17. Możejko, P.; Ptasińska-Denga, E.; Domaracka, A.; Szmytkowski, C. Absolute total cross-section measurements for electron collisions with tetrahydrofuran. *Phys. Rev. A* **2006**, *74*, 012708. [CrossRef]
- 18. Fuss, M.; Muñoz, A.; Oller, J.C.; Blanco, F.; Almeida, D.; Limão-Vieira, P.; Do, T.P.D.; Brunger, M.J.; García, G. Electron-scattering cross sections for collisions with tetrahydrofuran from 50 to 5000 eV. *Phys. Rev. A* **2009**, *80*, 052709. [CrossRef]
- Baek, W.Y.; Bug, M.; Rabus, H.; Gargioni, E.; Grosswendt, B. Differential elastic and total electron scattering cross sections of tetrahydrofuran. *Phys. Rev. A* 2012, *86*, 032702. [CrossRef]

- 20. Singh, S.; Gupta, D.; Antony, B. Electron and positron scattering cross sections for propene. J. Appl. Phys. 2018, 124, 034901. [CrossRef]
- Gupta, D.; Choi, H.; Singh, S.; Modak, P.; Antony, B.; Kwon, D. C.; Song, M. Y.; Yoon, J. S. Total ionization cross section of cyclic organic molecules. J. Chem. Phys. 2019, 150, 064313. [CrossRef]
- Naghma, R.; Gupta, D.; Goswami, B.; Antony, B. Electron impact ionization cross sections for chlorinated and brominated methane and C_nH_{2n+1}Cl (where n = 2, 3, 4) molecules. *Int. J. Mass Spectrom.* 2014, 360, 39–44. [CrossRef]
- 23. Hanwell, M.D.; Curtis, D.E.; Lonie, D.C.; V.; ermeersch, T.; Zurek, E.; Hutchison, G.R. Avogadro: An advanced semantic chemical editor, visualization, and analysis platform. *J. Cheminform.* **2012**, *4*, 1–17. [CrossRef] [PubMed]
- 24. Computational Chemistry Comparison and Benchmark Database (CCCBDB). Available online: http://cccbdb.nist.gov (accessed on 13 April 2022).
- 25. Cox, H.L., Jr.; Bonham, R.A. Elastic electron scattering amplitudes for neutral atoms calculated using the partial wave method at 10, 40, 70, and 100 kV for Z = 1 to Z = 54. *J. Chem. Phys.* **1967**, *47*, 2599–2608. [CrossRef]
- Tomer, H.; Modak, P.; Sinha, N.; Antony, B. Electron impact scattering from pentane molecules and effect of isomerism on cross section. *Chem. Phys. Impact* 2021, *3*, 100032. [CrossRef]
- Tomer, H.; Modak, P.; Alam, M.J.; Ahmad, S.; Antony, B. Electron scattering from molecules relevant to Titan's atmosphere. *Int. J. Mass Spectrom.* 2021, 470, 116708. [CrossRef]
- 28. Hara, S. The scattering of slow electrons by hydrogen molecules. J. Phys. Soc. Jpn. 1967, 22, 710–718. [CrossRef]
- 29. Zhang, X.; Sun, J.; Liu, Y. A new approach to the correlation polarization potential-low-energy electron elastic scattering by He atoms. *J. Phys. At. Mol. Opt. Phys.* **1992**, *25*, 1893. [CrossRef]
- 30. Staszewska, G.; Schwenke, D.W.; Thirumalai, D.; Truhlar, D.G. Quasifree-scattering model for the imaginary part of the optical potential for electron scattering. *Phys. Rev. A* **1983**, *28*, 2740. [CrossRef]
- 31. Staszewska, G.; Schwenke, D.W.; Truhlar, D.G. Complex optical potential model for electron–molecule scattering, elastic scattering, and rotational excitation of H₂ at 10–100 eV. *J. Chem. Phys.* **1984**, *81*, 335–343. [CrossRef]
- Vinodkumar, M.; Limbachiya, C.; Antony, B.; Joshipura, K.N. Calculations of elastic, ionization and total cross sections for inert gases upon electron impact: Threshold to 2 keV. J. Phys. At. Mol. Opt. Phys. 2007, 40, 3259. [CrossRef]
- Blanco, F.; Garcia, G. Screening corrections for calculation of electron scattering from polyatomic molecules. *Phys. Rev. A* 2003, 317, 458–462. [CrossRef]
- 34. Joshipura, K.N.; Vinodkumar, M. Cross sections and other parameters of $e-H_2O$ scattering (E i \geq 50 eV). *Pramana* **1996**, 47, 57–63. [CrossRef]
- 35. Garcia, G.; Manero, F. Correlation of the total cross section for electron scattering by molecules with 10–22 electrons, and some molecular parameters at intermediate energies. *Chem. Phys. Lett.* **1997**, *280*, 419–422. [CrossRef]
- 36. Hirschfelder, J.O.; Curtiss, C. F.; Bird, R.B. Molecular theory of gases and liquids. *Physics Today* 1955, 8, 17. [CrossRef]
- Szmytkowski, C.; Domaracka, A.; Możejko, P.; Ptasińska-Denga, E.; Kwitnewski, S. Electron scattering by sulfur tetrafluoride (SF₄) molecules. J. Phys. At. Mol. Opt. Phys. 2005, 38, 745. [CrossRef]
- Goswami, B.; Antony, B.; Fritzsche, S. Electron impact scattering and calculated ionization cross sections for SF_x (x = 1–5) radicals. *Int. J. Mass Spectrom.* 2017, 417, 8–15. [CrossRef]
- Harland, P.W.; Vallance, C. Ionization cross-sections and ionization efficiency curves from polarizability volumes and ionization potentials. *Int. J. Mass Spectrom. Ion Process.* 1997, 171, 173–181. [CrossRef]