



Nafees Uddin <sup>1,2</sup>, Paresh Modak <sup>1</sup>, and Bobby Antony <sup>1,\*</sup>

- <sup>1</sup> Atomic and Molecular Physics Laboratory, Department of Physics, Indian Institute of Technology (Indian School of Mines) Dhanbad, Jharkhand 826004, India; nafeesuddin27@gmail.com (N.U.); paresh@ap.ism.ac.in (P.M.)
- <sup>2</sup> JIMS Engineering Management Technical Campus, 48/4 Knowledge Park III, Greater Noida 201306, India
- \* Correspondence: bobby@iitism.ac.in; Tel.: +91-947-019-4795

**Abstract:** The need for a reliable and comprehensive database of cross-sections for many atomic and molecular species is immense due to its key role in R&D domains such as plasma modelling, bio-chemical processes, medicine and many other natural and technological environments. Elastic, momentum transfer and total cross-sections of butanol and pentanol isomers by the impact of 6–5000 eV electrons are presented in this work. The calculations were performed by employing the spherical complex optical potential formalism along with single-centre expansion and group additivity rule. The investigations into the presence of isomeric variations reveal that they are more pronounced at low and intermediate energies. Elastic, total cross-sections (with the exception of n-pentanol) and momentum transfer cross-sections for all pentanol isomers are reported here for the first time, to the best of our knowledge. Our momentum transfer cross-sections for butanol isomers are in very good agreement with the experimental and theoretical values available, and in reasonable consensus for other cross-sections.

Keywords: electron scattering; integral cross sections; alcohols; isomeric effect; butanol; pentanol

# 1. Introduction

Recently, there has been a heightened interest in the study of higher alcohols for their significant role in industrial applications and research. Species such as butanol and pentanol are axial to the development of bio-fuels [1] and are the mainstay of all major proposed solutions to the looming world energy crisis. To understand the processes that follow the ignition of plasma and to model the spark ignition behaviour of such bio-fuels, many fundamental data are required that can be sourced from electron-scattering studies of these molecules [2]. Moreover, there is a pressing need for a reliable and comprehensive database of cross-sections for these species, as they play a key role in R&D domains such as plasma modelling [3], bio-chemical processes [4], health [5], environment [6], etc.

In the present times, the isomers of higher alcohols have also been seen as viable alternatives of their n-structure counterparts as bio-fuels [7]. Electron-scattering data, however, are scarcely available for such molecules. These data are also critical for the accurate modelling of planetary atmospheres [8]. In order to facilitate a complete dataset of cross-sections [9], we report the data for elastic ( $Q_{el}$ ), momentum transfer ( $Q_{mtcs}$ ) and total cross-sections ( $Q_t$ ) for butanol and pentanol isomers under the present theoretical study. This is in continuation to the theoretical calculations of total ionisation cross-sections ( $Q_{ion}$ ) for the same species, reported in our earlier work [10].

Our calculations were performed using the spherical complex optical potential (SCOP) [11,12] methodology and the group additivity rule (GAR) [13], along with singlecentre expansion applied to model the charge density of each group, efficiently. A visual approach to the selection of groups on the basis of the electrostatic potential surface of the target molecule was employed, the details of which are provided in ref. [10]. The



Citation: Uddin, N.; Modak, P.; Antony, B. On the Electron Impact Integral Cross-Sections for Butanol and Pentanol Isomers. *Atoms* **2021**, *9*, 43. https://doi.org/10.3390/ atoms9030043

Academic Editor: Grzegorz Piotr Karwasz

Received: 8 June 2021 Accepted: 9 July 2021 Published: 13 July 2021

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



**Copyright:** © 2021 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/).



input parameters such as polarizability, ionisation energies, etc., for pentanol isomers were also calculated in our earlier work [10], though the first excited states of the targets were calculated in this work, the data being unavailable for the same in the literature. The next section describes our theoretical methodology followed by results and discussions with conclusions presented in the final section of this article.

### 2. Theoretical Methodology

We used the SCOP [14] formalism for the calculation of cross-sections that employ a model optical potential to represent the scattering dynamics, expressed as:

$$V_{opt} = V_{real}(r, E_i) + iV_{im}(r, E_i)$$
<sup>(1)</sup>

The Schrödinger equation for the system was then solved by the partial wave analysis using the potential in Equation (1), yielding the solutions as complex phase shifts that are used to obtain cross-sections. The potential represented by the first term on the right-hand side of Equation (1) is the sum of static potential ( $V_{st}$ ), exchange potential ( $V_{ex}$ ) and polarization potential ( $V_{pol}$ ).

$$V_{real} = V_{st} + V_{ex} + V_{pol} \tag{2}$$

The static potential was derived from the charge density ( $\rho$ ) of the atomic constituents of the target molecule where  $\rho$  is expanded about the scattering centre, which is the atom in case of atomic targets. In our case, however, the targets are molecules with hydrogen atoms attached to either a carbon atom or an oxygen atom, which are much heavier than the hydrogen itself. Consequently, the charge density of the hydrogen atom is expanded about the heavier atom, i.e., the carbon or the oxygen atom. This is called single-centre expansion. Due to the large size of our targets, it is fair to assume that they are composed of multiple independent scattering centres, comprising groups of atoms. The contributions of singleelectron collisions from these groups may be added linearly to obtain the cross-section for the whole molecule, a process that is known as the group additivity rule. To remove any ambiguity in the identification of these groups, we devised a selection mechanism based on the electrostatic potential surface of the molecule, described in our earlier work [10].

The static potential was obtained from the parameterized Hartree–Fock wave equation by Cox and Bonham [15], while the exchange potential was calculated using Hara's [16] non-parametric, free-electron gas model. The parameter-free, correlation polarization potential by Zhang et al. [17] was used to account for the polarization effects.

The second term on the right-hand side of Equation (1) corresponds to the loss of scattered flux due to electronic excitation and ionization channels. The absorption potential is a quasi-free Pauli-blocking type and its expression as given by Staszewska et al. [18] is:

$$V_{abs}(r, E_i) = -\rho(r)\sqrt{\frac{T_{loc}}{2}} \left(\frac{8\pi}{10k_F^3 E_i}\right) \theta(p^2 - k_f^2 - 2\Delta)(A_1 + A_2 + A_3)$$
(3)

Here, the local kinetic energy is:

$$T_{loc} = E_i - (V_{st} + V_{ex} + V_{pol}) \tag{4}$$

where  $k_f$  is the Fermi wave vector given by  $k_f = \sqrt[3]{3\pi^2\rho(r)}$  and p is the momentum of the incident electron computed as  $p^2 = 2E_i$ . The dynamic functions  $A_1$ ,  $A_2$  and  $A_3$ are dependent on the ionisation potential (IP), the Heaviside unit step function  $\theta(x)$  and the  $\Delta$  parameter, the value of which is such that it limits the value of the total inelastic cross-section. As approximated by Staszewska, the value of  $\Delta$  is equal to IP, which is a constant. The inelastic channels are closed for incident energies lower than  $\Delta$ , but below the ionization threshold, however, there is a finite probability of excitation to discrete states. An energy dependent form of  $\Delta$  checks the excessive loss of flux into the inelastic channels at intermediate energies, which is represented as:

$$\Delta(E_i) = 0.8I + \beta(E_i - I) \tag{5}$$

The constant  $\beta$  is calculated by setting  $\Delta = I$  (ionization energy) for  $E_i = E_p$ ,  $E_p$  being the incident energy where the inelastic cross-section is maximum. It is fair to consider the inelastic channels to be opened at the first excitation energy requiring energy dependency of  $\Delta$ . For energies higher than  $E_p$ , however,  $\Delta$  is fixed at ionization energy.

The optical potential constructed in Equation (1) for the target molecular system was incorporated in the Schrödinger equation, which was solved numerically using Numerov's method under partial wave analysis. The solutions yielded complex phase shifts, which carry information about scattering dynamics and were employed to calculate relevant cross-sections. The elastic cross-section for *l* partial waves is calculated as:

$$Q_{el}(E_i) = \frac{\pi}{k^2} \sum_{l=0}^{\infty} (2l+1) |\eta_l exp(Re\delta_l) - 1|^2$$
(6)

and the inelastic cross-section is given by:

$$Q_{inel}(E_i) = \frac{\pi}{k^2} \sum_{l=0}^{\infty} (2l+1) \left(1 - \eta_l^2\right)$$
(7)

where,  $\eta_l = exp(-2lm\delta_l)$  is the absorption factor for each partial wave with the number of partial waves, in our case being capped at 61, satisfying convergence of the results in our calculations. The sum of Equations (6) and (7) gives the total cross-section ( $Q_t$ ), i.e.:

$$Q_t = Q_{el} + Q_{inel} \tag{8}$$

The complex phase shifts obtained as the solutions of Schrödinger equation were also used to calculate the momentum transfer cross-section using:

$$Q_{mtcs}(E_i) = \frac{4\pi}{k^2} \sum_{l=0}^{\infty} (l+1) \sin^2[\delta_{l+1}(k) - \delta_l(k)]$$
(9)

We used the same data for target parameters, calculated by us or otherwise, as in our earlier work [10] and is displayed in Tables 1 and 2. This includes ionisation energies (IP) and molecular polarizabilities.

The excitation energies listed in Tables 1 and 2 were calculated using Gaussian software [19]. The geometry of the molecules was optimized using the hybrid functional (B3LYP) along with 6-311++G (d,) basis set within density functional theory [20,21]. Excited states calculations [22] were performed by implementing time dependent density functional theory on these optimized structures.

Table 1. Target properties (butanol isomers).

| Target Species      | IP (eV) [23]    | Polarizability<br>α (Å <sup>3</sup> ) | First Excited State<br>(eV) |
|---------------------|-----------------|---------------------------------------|-----------------------------|
| Butan-1-ol          | $9.99 \pm 0.05$ | 8.57 [24]                             | 6.23                        |
| Butan-2-ol          | $9.88\pm0.03$   | 8.57 [24]                             | 6.29                        |
| 2-methylpropan-1-ol | $10.02\pm0.03$  | 8.92 [25]                             | 6.24                        |
| 2-methypropan-2-ol  | $9.90\pm0.03$   | 8.92 [25]                             | 6.23                        |

| Target Species     | IP (eV) [10] | Polarizability<br>α (Å <sup>3</sup> ) [10] | First Excited State<br>(eV) |
|--------------------|--------------|--|-----------------------------|
| Pentan-1-ol        | 10.00        | 10.118                                     | 6.25                        |
| Pentan-2-ol        | 9.78         | 10.112                                     | 6.30                        |
| Pentan-3-ol        | 9.78         | 10.056                                     | 6.30                        |
| 2-methylbutan-1-ol | 9.86         | 10.000                                     | 6.20                        |
| 3-methylbutan-2-ol | 9.88         | 10.014                                     | 6.19                        |

Table 2. Target properties (pentanol isomers).

## 3. Results and Discussion

The calculated cross-sections of molecules are represented graphically (Figures 1–13). Atomic units were used for calculations with the cross-section values in the units of  $Å^2$  on the *Y*-axis and energy of the projectile in eV on the *X*-axis (logarithmic scale on both axes). Comparison data for the molecules are plotted in separate figures and, wherever it is not available, calculated data of all isomers of the target molecule are plotted in the same graph.



**Figure 1.** Elastic cross-section of butan-1-ol: solid black line represents present result, solid circles (red) depict experimental data from Khakoo et al., dashed (blue) line is ICS from Gomes et al., dash-dot line (green) is from Bhardvaja et al. and pink dash-dot-dot line represents pseudopotential calculations from Khakoo et al.



**Figure 2.** Solid lines (black) represent butan-2-ol, dashed lines (red) represent 2-methylpropan-1-ol and dotted lines (blue) represent 2-methylpropan-2-ol results. Lines (only) show present results and lines with open circles are results from Bettega et al.



**Figure 3.** Elastic cross-section of pentan-1-ol: solid black line shows present results, dashed blue line displays results by de Oliviera et al. and dash-dot red line represents results by Bhardvaja et al.



**Figure 4.** Elastic cross-section of pentanol isomers (present): black dashed line is for pentan-1ol, purple dotted line represents pentan-2-ol, red dash-dot-dot line represents pentan-3-ol, violet dash-dot line represents 2-methylbutan-1-ol and green solid line represents 3-methylpropan-2-ol.



**Figure 5.** Total cross-section butan-1-ol: black solid line shows present results, red circles are experimental results by Gomes et al., purple squares are 'hybrid TCS' by Gomes et al., blue dashed lines are calculated values by Gomes et al., green dash-dot-dot line is from Bhardvaja et al. and orange dash-dot-dash line shows TCS + rotational from Gomes et al.



**Figure 6.** Total cross-section of butanol isomers (present): solid (black) line represents butan-1-ol, dashed (olive) line is for butan-2-ol, dash-dot (red) line is for 2-methylpropan-1-ol and dash-dot-dot (blue) line represents 2-methylpropan-2-ol.



**Figure 7.** Total cross-section pentan-1-ol: solid (black) line represents present results and dashed (red) line represents results by Bhardvaja et al.



**Figure 8.** Total cross-section of pentanol isomers (present): dashed (black) line represents penta-1-ol, dotted (purple) is for pentan-2-ol, dash-dot-dot (red) line is for pentan-3-ol, dash-dot (blue) line represents 2-methylbutan-1-ol and solid (olive) line represents 3-methylbutan-2-ol results.



**Figure 9.** Momentum transfer cross-section of butan-1-ol: solid (black) line shows present results, circles (red) represent experimental results of Khakoo et al. and dashed (pink) line shows calculated results of Bettega et al.



**Figure 10.** Momentum transfer cross-section of butanol isomers (present): solid (black) line represents butan-1-ol, dashed (olive) line is for butan-2-ol, dash-dot (red) line is for 2-methylpropan-1-ol and dash-dot-dot (blue) line represents 2-methylpropan-2-ol.



**Figure 11.** Momentum transfer cross-section for butanol isomers: present results are depicted as lines and results from Bettega et al. are shown as lines with open circles. Butan-2-ol results are shown in black, 2-methylpropan-1-ol in red and 2-methypropan-2-ol results in blue colour.



**Figure 12.** Momentum transfer cross-section of pentan-1-ol: solid (black) line shows present results, dashed (blue) lines show calculated (SE) results of de Oliviera et al. and dash-dot (red) line represents calculated (SEP) results of de Oliviera et al.



**Figure 13.** Momentum transfer cross-section of pentanol isomers: dashed (black) line represents penta-1-ol, dotted (purple) is for pentan-2-ol, dash-dot-dot (red) line is for pentan-3-ol, dash-dot (blue) line represents 2-methylbutan-1-ol and solid (olive) line represents 3-methylbutan-2-ol results.

### 3.1. Elastic Cross-Section

Our elastic cross-section values for butan-1-ol (Figure 1) were on the higher side for lower energies (<10 eV) as compared to the experimental data of Khakoo et al. [26], their calculated results and that of Gomes et al. [27]. This may be inherent to our methodology and can be attributed to the fact that we considered inelastic channels open at the first excitation energy albeit there being no distinction between the various open channels. The number of scattering centres in straight chain isomers was larger than the branched ones in our implementation of group additivity rule [10], to which their higher cross-section values below the ionization threshold can be attributed. This, however, improved the overall results, especially in the context of contribution to energies above the ionisation threshold. The agreement with experimental results at intermediate energies, therefore, was reasonable within the given stated range of uncertainties. Just above the ionization threshold, present data points overestimate the reported results since the inner excitations were not included in the present case. These inner excitations were dominating inelastic channels besides the ionization above the ionization threshold. Therefore, elastic cross-

section reduces significantly just above the ionization threshold. Our results (Figure 2) show a distinct difference in the elastic cross-sections of straight chain isomers as compared to the branched ones, and the same can be observed in the results of Bettega et al. [28] too, although the difference in their case is marginal. It is noteworthy here, that the branched isomers of alcohols are polar molecules due to the presence of hydroxyl group. This effect is mitigated for straight chain isomers.

The integral elastic cross-sections of pentan-1-ol reported by de Oliviera et al. [29] have higher values at intermediate energies than calculated elastic cross-sections of Bhardvaja et al. [30] and our results (Figure 3), though the trends appear similar. The effect of the isomeric structure on the elastic cross-section of pentanol isomers, however, appears to be of minor significance in our results (Figure 4) except for 3-methylbutan-2-ol. This deviation from the trend in comparison with butanol isomers needs more investigation, as this secondary amyl alcohol has a methyl group as well as a hydroxyl group attached to the inner carbon atoms.

#### 3.2. Total Cross-Section

The experimental total cross-section (TCS) for butan-1-ol reported by Gomes et al. [27] in the energy range 80–400 eV starts off higher than all theoretically calculated cross-sections, including their own and falls of more rapidly approaching 400 eV. All theoretical calculations, more or less, show an identical trend in results, though differing in magnitude. Our results are in excellent agreement with experimental data between 250 and 400 eV. Gomes et al. [27] derived a 'hybrid TCS' from the elastic integral cross-section of Khakoo et al. and the calculated total ionization cross-section of Ghosh et al. [31] by adding Binary-Encounter-Bethe (BEB) with an implementation of outer valence Green's function (OVGF), which is shown in (Figure 5). Given the fact that there is a difference in magnitude of the 'hybrid TCS' and experimental TCS of Gomes et al. [27], it is noteworthy that our results at the lower end of intermediate energies are in good agreement with the former and at the higher end with the latter. A comparison of total cross-sections of butanol isomers (Figure 6) continues to display the trend observed in the case of our results for their elastic cross-sections.

Our calculated TCS of pentan-1-ol (Figure 7) is in very good agreement with the calculated results of Bhardvaja et al. [30], except for very low and very high energies. There are no experimental results available for the same to the best of our knowledge for comparison with our data. Interestingly, the TCS results of pentanol isomers (Figure 8) inherited the same features from their elastic cross-sections and here again, 3-methylbutan-2-ol displays a deviation from the trend observed in butanol isomers.

#### 3.3. Momentum Transfer Cross-Section

The  $Q_{mtcs}$  results of butan-1-ol from our calculations (Figure 9) are in excellent agreement with experimental results of Khakoo et al. [26] and the theoretical results of Bettega et al. [28]. Here again our results below 10 eV were quite high as compared to the other two. The reason is same as for the elastic curve.

As far as a comparison of our  $Q_{mtcs}$  results for butanol isomers (Figure 10) is concerned, they showed a similar trend as  $Q_{el}$  and  $Q_t$ , i.e., the values were higher in magnitude for straight chain isomers than the branched ones. The agreement, when compared with calculated results (Figure 11) of Bettega et al. [28], is in parts and is better for butan-2-ol.

There are no experimental data available for pentan-1-ol to the best of our knowledge, hence, we compared the present results (Figure 12) with static-exchange and static-exchange plus polarization calculations of de Oliviera et al. [29], which are in very good agreement with our results except for energies lower than the ionisation threshold. Since there is no experimental or theoretical data available for  $Q_{mtcs}$  of isomers except for pentan-1-ol, a comparison of our results (Figure 13) shows that they are in line with the observations for our elastic and total cross-sections. The isomer effect here again is not significant for the ones other than 3-methylbutan-2-ol, which has values higher in magnitude in low

to intermediate energy range as compared to others. The trend shown by all isomers, however, is consistent and along expected lines.

# 4. Conclusions

Electron-scattering elastic, total and momentum transfer cross-sections for butanol and pentanol isomers were calculated and presented in this study. The SCOP method was employed for the calculations. Taking into consideration the large size of the molecules, the group additivity rule was used with scattering centres identified based on the electrostatic potential surface generated for each target. The first excited states were calculated for all the target species and cross-sections are reported for incident electron energies ranging from 6 to 5000 eV. With this dataset, the cross-section database is complete for both butanol and pentanol isomers. While our elastic and total cross-sections for most target isomers are in good agreement with available measured and/or calculated results, our momentum transfer cross-section calculations are in excellent agreement with available data for butan-1-ol. There was a small but significant difference observed in the cross-sections of straight chain and branched isomers, although the trends are contrary for butanol and pentanol, which is not appreciable at higher energies.

**Author Contributions:** N.U. and B.A. conceived of the presented idea. N.U. performed the computations. P.M. assisted with calculations. B.A. supervised the work. All authors discussed the results and contributed to the final manuscript. All authors have read and agreed to the published version of the manuscript.

Funding: This research received no external funding.

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

Conflicts of Interest: The authors declare no conflict of interest.

## References

- 1. Erdiwansyah; Mamat, R.; Sani, M.; Sudhakar, K.; Kadarohman, A.; Sardjono, R. An overview of higher alcohol and biodiesel as alternative fuels in engines. *Energy Rep.* 2019, *5*, 467–479. [CrossRef]
- Lopes, M.C.A.; Silva, D.G.M.; Bettega, M.H.F.; da Costa, R.F.; Lima, M.A.P.; Khakoo, M.A.; Winstead, C.; McKoy, V. Low Energy Electron Scattering from Fuels. J. Phys. Conf. Ser. 2012, 388, 012014. [CrossRef]
- 3. Ridenti, M.; Filho, J.; Brunger, M.; Lima, M.P. Electron scattering by biomass molecular fragments: Useful data for plasma applications? *Eur. Phys. J. D.* 2016, 70, 16. [CrossRef]
- 4. Boudaïffa, B.; Cloutier, P.; Hunting, D.; Huels, M.A.; Sanche, L. Resonant formation of DNA strand breaks by low-energy (3 to 20 eV) electrons. *Science* **2000**, *287*, 1658–1660.
- 5. Sanz, A.G.; Fuss, M.C.; Muñoz, A.; Blanco, F.; Limão-Vieira, P.; Brunger, M.J.; Buckman, S.J.; Garcia, G. Modelling low energy electron and positron tracks for biomedical applications. *Int. J. Radiat. Biol. Inf. UK Ltd.* **2011**, *88*, 71–76. [CrossRef]
- 6. Joshipura, K.N.; Antony, B.; Vinodkumar, M. Electron scattering and ionization of ozone, O2and O4molecules. J. Phys. B At. Mol. Opt. Phys. 2002, 35, 4211–4221. [CrossRef]
- Sarathy, S.M.; Park, S.; Weber, B.; Wang, W.; Veloo, P.S.; Davis, A.C.; Togbe, C.; Westbrook, C.K.; Park, O.; Dayma, G.; et al. A comprehensive experimental and modeling study of iso-pentanol combustion. *Combust. Flame* 2013, 160, 2712–2728. [CrossRef]
- Campbell, L.; Brunger, M. Electron collisions in atmospheres. *Int. Rev. Phys. Chem.* 2016, *35*, 297–351. [CrossRef]
   Tanaka, H.; Brunger, M.J.; Campbell, L.; Kato, H.; Hoshino, M.; Rau, A.R.P. Scaled plane-wave Born cross sections for atoms and
- molecules. *Rev. Mod. Phys.* 2016, 88, 025004. [CrossRef]
- Uddin, N.; Verma, P.; Alam, M.J.; Ahmad, S.; Antony, B. Electron impact total ionization cross section for C4 and C5 isomeric alcohols. *Int. J. Mass Spectrom.* 2018, 431, 37–42. [CrossRef]
- 11. Jain, A. Electron scattering with methane molecules at 20–500 eV. J. Chem. Phys. 1984, 81, 724–728. [CrossRef]
- 12. Joshipura, K.N.; Patel, P.M. Total electron scattering cross sections for NO, CO, and eV). J. Phys. B At. Mol. Opt. Phys. 1996, 29, 3925–3932. [CrossRef]
- 13. Joshipura, K.N.; Vinodkumar, M. Various total cross-sections for electron impact on. Eur. Phys. J. D. 1999, 5, 229.
- 14. Antony, B.; Joshipura, K.; Mason, N. Electron impact ionization studies with aeronomic molecules. *Int. J. Mass Spectrom.* 2004, 233, 207–214. [CrossRef]
- 15. Cox, H.L.; 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]
- 16. Hara, S. The Scattering of Slow Electrons by Hydrogen Molecules. J. Phys. Soc. Jpn. 1967, 22, 710–718.

- 17. Zhang, X.; Sun, J.; Liu, Y. A new approach to the correlation polarization potential-low-energy electron elastic scattering by the atoms. *J. Phys. B At. Mol. Opt. Phys.* **1992**, 25, 1893–1897. [CrossRef]
- 18. 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*, 2740–2751. [CrossRef]
- Frisch, M.J.; Trucks, G.W.; Schlegel, H.B.; Scuseria, G.E.; Robb, M.A.; Cheeseman, J.R.; Scalmani, G.; Barone, V.; Petersson, G.A.; Nakatsuji, H.; et al. Gaussian<sup>~</sup>09 Revision, C.01. Available online: <a href="https://gaussian.com/g09citation/">https://gaussian.com/g09citation/</a> (accessed on 1 August 2020).
- 20. Becke, A.D. Density-functional exchange-energy approximation with correct asymptotic behavior. *Phys. Rev. A* **1988**, *38*, 3098–3100. [CrossRef]
- 21. Lee, C.; Yang, W.; Parr, R.G. Development of the Colle-Salvetti correlation-energy formula into a functional of the electron density. *Phys. Rev. B* **1988**, *37*, 785–789. [CrossRef]
- Faizan, M.; Afroz, Z.; Alam, M.J.; Rodrigues, V.; Ahmad, S.; Ahmad, A. Structural, vibrational and electronic absorption characteristics of the monohydrate organic salt of 2-amino-5-bromo-6-methyl-4-pyrimidinol and 2,3-pyrazinedicarboxylic acid: A combined experimental and computational study. J. Mol. Struct. 2019, 1177, 229–241. [CrossRef]
- 23. Computational Chemistry Comparison and Benchmark DataBase Release 21 (August 2020) Standard Reference Database 101 National Institute of Standards and Technology. Available online: http://cccbdb.nist.gov/ (accessed on 1 August 2020).
- 24. Gussoni, M.; Rui, M.; Zerbi, G. Electronic and relaxation contribution to linear molecular polarizability. An analysis of the experimental values. *J. Mol. Struct.* **1998**, 447, 163–215. [CrossRef]
- 25. Haynes, W.M. CRC Handbook of Chemistry and Physics, 95th ed.; Haynes, W.M., Ed.; CRC Press: Boca Raton, FL, USA, 2014.
- 26. Khakoo, M.A.; Muse, J.; Silva, H.; Lopes, M.C.A.; Winstead, C.; McKoy, V.; De Oliveira, E.M.; Da Costa, R.F.; Varella, M.; Bettega, M.; et al. Elastic scattering of slow electrons byn-propanol andn-butanol. *Phys. Rev. A* **2008**, *78*, 062714. [CrossRef]
- Gomes, M.; da Silva, D.G.M.; Fernandes, A.C.P.; Ghosh, S.; Pires, W.A.D.; Jones, D.B.; Blanco, F.; García, G.; Brunger, M.J.; Lopes, M.C.A. Electron scattering from 1-butanol at intermediate impact energies: Total cross sections. *J. Chem. Phys.* 2019, 150, 194307. [CrossRef] [PubMed]
- 28. Bettega, M.; Winstead, C.; McKoy, V. Low-energy electron scattering fromC4H9OH isomers. *Phys. Rev. A* 2010, *82*, 062709. [CrossRef]
- 29. De Oliveira, E.M.; do N Varella, M.T.; Bettega, M.H.F.; Lima, M.A.P. Elastic scattering of slow electrons by n-pentanol alcohol. *Eur. Phys. J. D* **2014**, *68*, 65. [CrossRef]
- 30. Bharadvaja, A.; Kaur, S.; Baluja, K.L. Study of electron collision from bioalcohols from 10 to 5000 eV. *Eur. Phys. J. D* 2019, 73, 251. [CrossRef]
- Ghosh, S.; Nixon, K.; Pires, W.; Amorim, R.; Neves, R.; Duque, H.; da Silva, D.; Jones, D.; Blanco, F.; Garcia, G.; et al. Electron impact ionization of 1-butanol: II. Total ionization cross sections and appearance energies. *Int. J. Mass Spectrom.* 2018, 430, 44–51. [CrossRef]