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Research Article

Molecular Orientation Resolved (e, 2e) Cross Sections for CF_4 at 67 eV Impact Energy

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Abstract

In this investigation, the fully differential cross sections (FDCS) for ionization of electron impact at low energy (E_0 = 67 eV) were measured for the specific orientations of the molecules and around it axis. In the full perpendicular plane (FPP), the FDCS for CF_4 were experimentally figured out by using reaction microscope (REMI) for different kinematics such as two ejection electron energies of 5 eV and 8 eV, scattering angles of -25° and 30°, and two molecular axis directions of ϕ_{Mol} = 0 °and 45 °, also their relative orientations such as 180 °and 225 °. The momentum vectors of the two ejected electrons (with energies E_{e1}, and E_{e2}) and the fragment ions (e, 2e+ ions) were detected by the triple coincidence method. For the duration of dissociation, the time of flight (TOF) of CF_3^+, CF_2^+, CF^+, F^+, and C^+ are observed in the TOF diagram. During the dissociation of the final fragment of CF_3^+ ion and its electronic ground state neutral F, the momentum vector of CF_3^+ allows us to draw conclusions about the orientation of the molecule in the course of the collision. Finally, it was remarked that concerning molecular orientation, electrons are highly sensitive at low energy and low scattering angle.

Keywords

Electron-Impact Ionization (EII), FDCS, Molecular Orientation, REMI and Full Perpendicular Plane

1. Introduction

In Physics, the ionization of atoms and molecules by electrons is of significant attention today to both theoretical and experimental aspects. It plays an essential role in several scientific and practical applications, ranging from radiation chemistry and biology to astrophysics and atmospheric sciences [1, 2]. For instance, it has recently been discovered that low-energy electrons can induce DNA strand breaks and cluster destruction through electron dissociation resonance and the superposition of different excitation-dissociation and ionization mechanisms involved in the process [3-5]. It is

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therefore so crucial in the treatment of cancer. The alignment and orientation of the molecular axis relative to the momentum of the incident projectile must be suitable for multiple- or higher-order scattering of the two active electrons in the molecule. Apart from that, for Young's double-slit interference which can occur owing to electron scattering through two indistinguishable centers, molecular bonding and orientation will determine the pattern of observed interference.

For simple molecules such as H_2, O_2, and N_2, only a few (e,2e) experiments have been able to successfully resolve the orientation of the molecular axis cross-section in the bygone. This was achieved by studying the reaction in which the H_2^+ ion dissociates in the electronic ground state [2, 3] or in an excited state [4], and the direction of proton release allows conclusions to be drawn about the orientation of the molecular axis.

For larger systems (molecules such as CF_4, CH_4, CO_2, H_2O, etc.), it is perplexing to study the dynamics of small bodies during EII. The few-body problem is one of the most fundamental unsolved problems in physics. It arises from the fact that the Schrödinger equation for complex molecules cannot be solved analytically for more than two interacting particles. A kinetically complete study of electron impact ionization on atoms and molecules provides detailed insights into correlated small body reactions. Therefore, for more than two particles, approximations must be made or the problem must be addressed iteratively by further experimental studies and theoretical calculations. Tetrafluoromethane (CF_4) has tetrahedral symmetry and is relevant to many scientific and practical fields, with many unsolved problems in molecular physics [6-8].

Here, the resolved (e, 2e) molecular orientation cross section of CF_4 is studied at an impact energy of 67 eV in a full perpendicular plane which is perpendicular to the incident projectile direction. The polar angle of the ejected electron is fixed at $\theta_{Mol} = 90°$ and the azimuthal angle ϕ_{e2} is varied from 0 ° to 360 °. In this plane, the entire angular range of ϕ_{e2} is experimentally accessible.

The electrons from certain orbitals of atoms or molecules are quite sensitive to ionization as always. If a molecule is oriented around its axis during ionization (the orientation changes by 180 °), we can be able toss observe how the emission pattern of the emitted electrons differs in cross sections before and after the orientations, which was the main objective of this study.

2. Materials and Methods

The experiment is carried out by using a reaction microscope (REMI), and the experimental approach is often designed for the kinetic study of electron-atom or electron-molecule collision investigations, in which the energy and direction of all charged particles in their final state are determined.

The basic principle of a general REMI was described by Ullrich and his colleagues [6]. As shown in Figure 1, the particulars of the investigational techniques are described in previous studies [7, 8, 14]. The core points of the experimental method are listed below. A well-focused (diameter about 1 mm) pulsed electron beam of a specific energy passes through a supersonic gas jet. The target gas expands through a nozzle with a diameter of 30 μm, throughout the two skimmers and lastly enters the main scattering chamber. A photoelectron gun was used in which a tantalum photocathode is irradiated with a pulsed ultraviolet laser with a wavelength of 266 nm (about 4.67 eV) and a pulse width of less than 0.5 ns. The generated electrons are accelerated to form a pulsed electron beam of the required energy, which collides with the molecular beam at a 90 °angle. After the collision, the charged particles (two electrons and one ion) are accelerated and directed by uniform electric and magnetic fields, detected by opposing electron and ion detectors finally. In this experiment, data were obtained using the triple coincidence (e, 2e + ion) method, which detects two exiting electrons (with energies E_1 and E_2) and ion products. The experimental data were collected in the laboratory of the MPINP in Heidelberg. The time of flight (TOF) and the position of the particle on the detector are measured. Electrons in the spectrometer are accelerated by a uniform electric field with a length a_e = 11 cm from the interaction region and fly into a drift region (field-free space) with a length d_e = 22 cm.

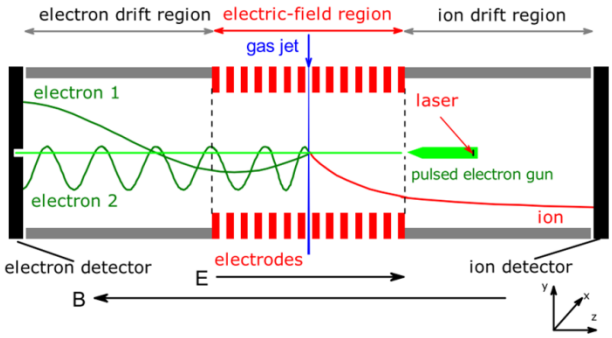

Figure 1. *Schematic diagram of reaction microscope is used to study EII and molecular breakup [7].*

According to the time focusing condition, $2a_e = d_e$. The acceleration and drift lengths of the ions are a_i = 6.8 cm and d_i = 13.6 cm, respectively. From the raw data after offline calibration with the analysis software Go*4* based on C and C^{++} programs, the momentum vector of each particle can be determined. The solid angle of electron detection is almost 4π. For the dissociation process, the fully differential cross section of the ion CF_3^+ can be measured. The direction of CF_3^+ (dissociation) allows the determination of molecular alignment and orientation. The determination of molecular alignment and orientation is based on the axial recoil approximation using the detected CF_3^+ pulse. The time of flight of CF_3^+, CF_2^+, CF^+, F^+, and C^+ are shown in Figure 2.

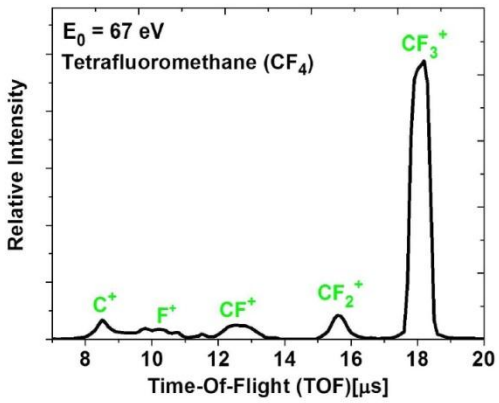

Figure 2. *Ion time of flight [14].*

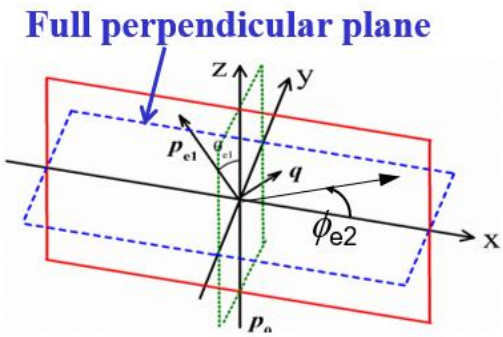

Figure 3. *Three planes (i) the scattering (xz) plane (red solid frame), (ii) the perpendicular (yz) plane (green dotted), and (iii) the full perpendicular (xy) planes (blue dashed).*

3. Results and Discussion

CF_4 molecule is a non-hydrogenic polyatomic molecule and has tetrahedral geometry. The ground state electronic configuration of the CF_4 molecule (in T_d symmetry) is given by [14]

$$\underbrace{(1a_1)^2(1t_2)^6}_{F1s}\underbrace{(2a_1)^2}_{C1s}\underbrace{(3a_1)^2(2t_2)^6}_{inner-valence}\underbrace{(4a_1)^2(3t_2)^6(1e)^4(4t_2)^6(1t_1)^6}_{outer-valence}\ {}^1A_1$$

The two lowest unoccupied orbitals (LUMOs) in the ground state of this molecule are $5a_1$ and $5t_2$. The five outer-valence orbitals are $1t_1$, $4t_2$, 1e, $3t_2$, and $4a_1$ and their vertical ionization energies are known from high-resolution HeI and HeII Photoelectron Spectra (PES) to be 16.20, 17.40, 18.50, 22.12 and 25.12 eV respectively and the vertical ionization energies of the inner-valence orbitals ($2t_2$, $3a_1$) are 40.3eV and 43.8 eV respectively [14]. The three highest occupied molecular orbitals (HOMOs) are the lone-pair orbitals of the fluorine atoms and lie within 2.3 eV of each other. Ionizing one electron from the outer-valence orbitals with increasing binding energy will lead to CF_4^+ in the ionic states $\tilde{X}\ {}^2T_1$, $\tilde{A}\ {}^2T_2$, $\tilde{B}\ {}^2E$, $\tilde{C}\ {}^2T_2$ and $\tilde{D}\ {}^2A_1$ [14].

3.1. Full Perpendicular Plane and kinematics

Figure 3 shows the scattering kinematics of the incident projectile with momentum p_0 along with z-axis, also the scattering projectile with momentum p_{e1} and scattering angle θ_{e1} which define the xz-plane (solid red line). The vertical (yz) plane and the perfectly vertical (xy) plane are marked with green (dotted) and blue (dashed) frames, respectively [9, 10]. The direction of momentum transfer is denoted by q. In these studies, FDCS is observed in a perfectly vertical plane (xy-plane) perpendicular to the incident projectile direction, with the polar angle of the emitted electron set to $\theta_{Mol} = 90°$ and the azimuthal angle ϕ_{e2} which varies from 0 ° to 360 °. In this plane, the full angular range of ϕ_{e2} can be accessed experimentally.

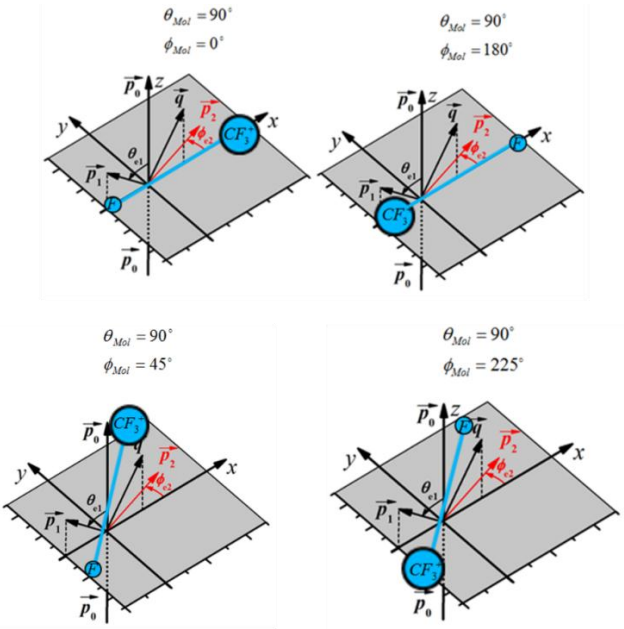

Figure 4. *Orientation of molecule during ionization.*

This paper summarizes the results of the fully differential cross sections at two different orientations in a full perpendicular plane (θ_{Mol} = 90 °), two emitted electron energies of 5 eV and 8 eV, and scattering angles of −25° and −30°, as well as the two molecular axis orientations of ϕ_{Mol} = 0 ° and 45 ° and their relative orientations [11-13], as shown in Figure 4.

3.2. The Fully Differential Cross Section (FDCS)

Figure 5 shows the FDCS for emitted electron energies of 5 eV and 8 eV, scattering angles of -25 °and -30 °, and molecular axis orientations of ϕ_{Mol} = 0 °and perfectly perpendicular 180 °. The cross sections are symmetric about 180 °. Binary and recoil peaks are observed near ϕ_{e2} = 0° and 180°, respectively [5, 13]. Due to the orientation, the FDCS near the recoil peak is observed to have a large discrepancy between ϕ_{Mol} = 0 °and 180 °for low energy kinematics and small scattering angles.

Figure 6 shows the FDCS for emitted electron energies of 5 eV and 8 eV, scattering angles of -25 ° and -30 °, and perfectly perpendicular molecular axis orientations of ϕ_{Mol} = 45 ° and 225 °. The cross sections are symmetric about 180 °. Binary and recoil peaks are observed near ϕ_{e2} = 0° and 180°, respectively. Due to the orientation, the FDCS near the recoil peak is observed to have a weak discrepancy in the range of ϕ_{Mol} = 45 ° to 225 ° for low energy kinematics and small scattering angles.

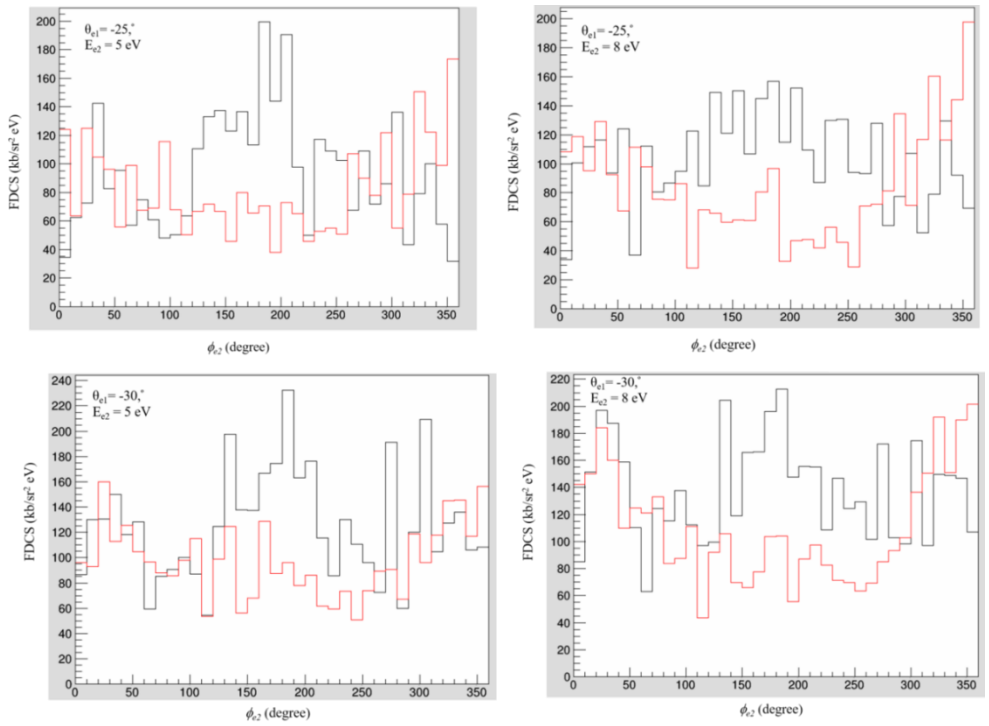

Figure 5. *FDCS for ionization of the CF_4 molecule with energies E_2 = 5 eV and 8 eV, molecular axis orientation ϕ_{Mol} = 0 °, and two fixed electron scattering angles θ_{e1} = -25 ° and -30 ° at a relative orientation of 180 °.*

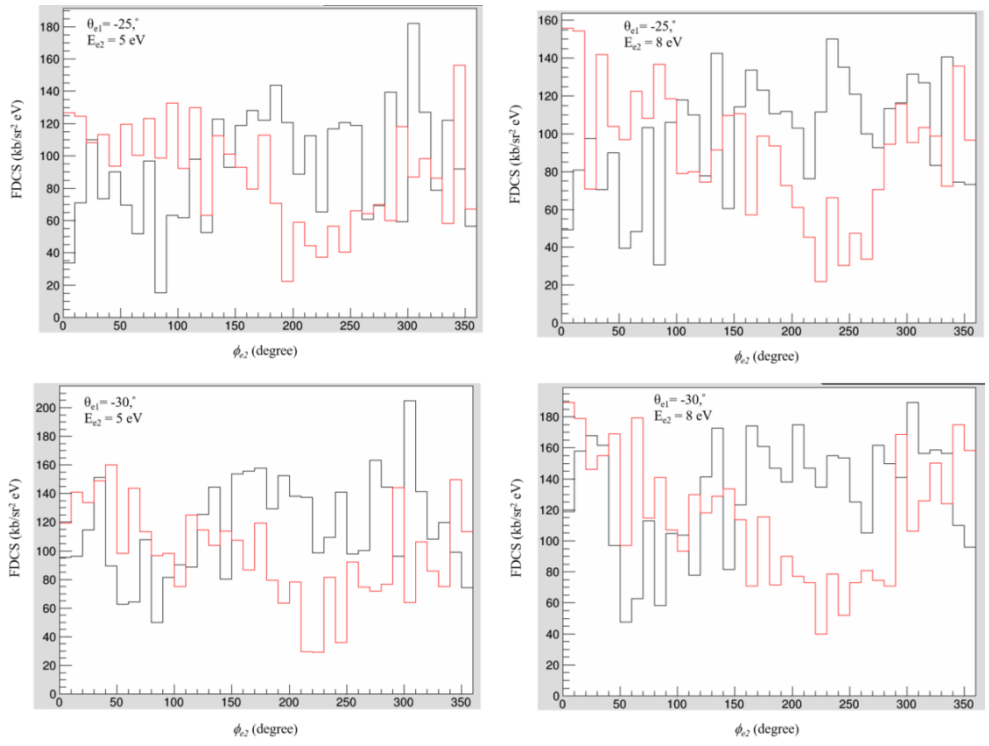

Figure 6. *FDCS for ionization of the CF_4 molecule with two fixed electron scattering angles θ_{e1} = -25 ° and -30 ° at energies E_2 = 5 eV and 8 eV, molecular axis orientation ϕ_{Mol} = 45 °, and relative orientation 225 °.*

4. Conclusions

An experimental study of electron impact ionization of CF_4 has been performed with an ejection energy of E_0 = 67 eV. The final state particle is determined using a reaction microscope for three-dimensional momentum vector, where experimental are the five outer valence orbitals $1t_1$, $4t_2$, 1e, $3t_2$, and $4a_1$ of the fully differential cross sections (FDCS). This outcome supports in a full perpendicularly stable CF_3^+ cation. The measured FDCS are cross-normalized over all scattering angles θ_1 from -25 ° to -30 ° and ejection electron energies of E_2 from 5 eV to 8 eV, also FDCS plots elucidate the position and intensity of the recoil peak and the binary peak, are strongly dependent on the orientation of molecules. According to these characteristics, the recoil peak arises from backscattering of the outgoing electrons in the molecular potential, which induces on focusing along the molecular axis. Thus, molecular orientation is highly sensitive to the electron emission pattern due to same kinematics particularly at low energy and low scattering angle such as 5 eV and -25 ° respectively.

Abbreviations

REMI	Reaction Microscope
FPP	Full Perpendicular Plane
FDCS	Fully Differential Cross Sections
EII	Electron-Impact Ionization
MPINP	Max Planck Institute for Nuclear Physics

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Author Contributions

Khokon Hossen: Conceptualization and Supervision
Humaira Takia: Validation
Hossain Mohammad Arshad: Writing-review & editing
Rahman Moshiur: Writing – review & editing
Md. Bellal Hossain: Writing – review & editing
Muhammad Masudur Rahaman: Writing-review & editing

Conflicts of Interest

The authors declare no conflicts of interest.

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