

Electron-impact total, multiple-differential elastic, and ionization cross sections of ammonia: A joint theoretical and experimental study

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Combined experimental and theoretical studies are performed on the elastic scattering and electron-impact ionization of ammonia (NH_3) in the energy range of 30 eV to 1 keV. Differential elastic scattering cross sections are measured across an angular range of 5° to 150° , while doubly differential ionization cross sections were measured in the angular range of 30° to 135° , with secondary electron energies ranging from 5 eV up to about half the primary electron energy. In parallel with the measurements, theoretical calculations of differential elastic scattering and doubly differential ionization cross sections of NH_3 are performed using the IAM-SCAR + I approach, the POLYDCS code, and the distorted wave Born approximation. Reasonably good agreement is observed between the present experimental results and theoretical predictions. Total ionization cross sections, derived by integrating the experimental doubly differential ionization cross sections over the emission angle and secondary electron energies, show excellent agreement with theoretical values obtained using the Binary-Encounter-Bethe model with rescaled orbital binding and mean kinetic energies, and are consistent with experimental data measured by another group using a different method. As a final validation, the sum of the total elastic and ionization cross sections is compared with the recommended total electron scattering cross sections, confirming the consistency of the present experimental results.

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I. INTRODUCTION

Ammonia (NH_3) has recently gained significant attention as a sustainable, carbon-free energy carrier. In contrast to hydrogen, NH_3 is easier to store and transport, and can be combusted without emitting carbon dioxide. It is also important for agriculture, serving as the primary precursor in the production of synthetic fertilizers. However, its industrial synthesis via the Haber-Bosch process remains highly energy-intensive and carbon dependent.

To overcome this challenge, nonthermal plasmas are explored for NH_3 production. These plasmas rely on energetic electrons, rather than high temperatures, to initiate chemical reactions. Accurate modeling of such plasmas requires detailed knowledge of electron- NH_3 interactions, including elastic scattering and ionization processes [1].

In addition to its industrial relevance, NH_3 is a dominant nitrogen species in Earth's atmosphere and is also present in various planetary environments. It plays a critical role

in aerosol nucleation, cloud formation, and can influence the ozone layer, thereby impacting climate dynamics. In both plasma and atmospheric applications, the availability of accurate electron-impact cross section data is essential for simulations and predictive modeling.

Beyond its environmental and industrial relevance, ammonia also holds biological significance. As the simplest molecule featuring a nitrogen-hydrogen (N-H) bond, NH_3 serves as a fundamental functional unit in various biomolecular systems.

Given NH_3 's importance across energy, environmental, and biological sciences, extensive research on electron- NH_3 collisions exist in the literature. However, as deduced from the comprehensive review by Itikawa [2], the dataset remains incomplete in key areas, particularly for angle-resolved ionization processes. This study aims to address several of these gaps.

The first experimental elastic electron scattering measurements on NH_3 were indirectly reported by Harshbarger *et al.* [3], who cited unpublished absolute differential cross sections (DCSSs) from Bromberg at incident energies 300 eV, 400 eV, and 500 eV and scattering angles below 10° . A more comprehensive dataset was published in 1992 by Alle *et al.* [4], covering absolute DCSSs, total elastic cross sections (TECS), and momentum transfer cross sections (MTCSSs) for energies of 2 eV to 30 eV and a broader angular range between 10° and 125° . This work was later

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extended by Homem *et al.* [5], who provided experimental and theoretical elastic scattering cross sections with similar scattering angles in the intermediate energy range of 50 eV to 500 eV.

Despite the importance of ionization data for plasma modeling, relatively few studies have reported angle-resolved electron-impact ionization cross sections. Triply differential cross sections (TDCSs) for all valence orbitals of NH_3 were measured by El Mir *et al.* [6,7] in 2015 and 2021, using a coplanar asymmetric geometry. These experiments were conducted at secondary electron energies of 12 eV, 37 eV, and 74 eV, with the scattered electron having an energy of 500 eV. Additionally, Rejoub *et al.* [8] published total ionization cross sections (TICSs) in 2001, and also provided partial ionization cross sections using a time of flight (TOF) technique. More recently, Choi *et al.* [9] reported total scattering cross sections (TCSs) in the energy range between 18.5 eV and 90 eV.

Recognizing the continued need of comprehensive and reliable cross section data, this study presents new measurements of both elastic and ionization differential cross sections. Specifically, experimental elastic DCS and their integrated quantities (TECS, MTCS) are reported over an incident energy range of $T = 30$ eV to 1 keV and scattering angles between 5° and 150° . These are complemented by theoretical results obtained using the IAM-SCAR + I method [10,11].

In addition, we report experimental doubly differential electron-impact ionization cross sections (DDCSs) of NH_3 over the same energy range and an angular range 30° – 135° , with secondary electron energies of 5 eV up to $(T - I)/2$, where $I = 10.07$ eV is the ionization potential of NH_3 [12]. The DDCS data were integrated over emission angle θ_e and secondary electron energy E to yield singly differential (SDCSs) and total ionization cross sections. Theoretical calculations based on the distorted wave Born approximation (DWBA) were also performed and compared to present experimental DDCS results.

II. EXPERIMENTAL PROCEDURE

The experimental setup and procedures used in this work have been described in detail previously ([13,14]), where we employed a crossed-beam configuration in combination with the relative flow technique. Therefore, only a brief overview of the measurement is given here.

Two different experimental setups were used, depending on whether elastic or ionization cross sections were being measured. Elastic scattering cross sections were obtained using the setup described in Ref. [14], which allows measurement over a wider angular range but with a lower signal-to-noise ratio, making it unsuitable for measurements of ionization processes with low cross sections. For ionization measurements, a separate setup [13] offering a better signal-to-noise-ratio was employed. To ensure consistency, the elastic scattering cross sections measured with both setups were compared and found to be in good agreement.

In both setups (see Fig. 1), a monoenergetic electron beam with an energy spread of less than 0.5 eV, produced by an electron gun, intersects perpendicularly with a molecular beam. The electron beam current is measured using a Faraday cup positioned beyond the nozzle. The molecular beam is

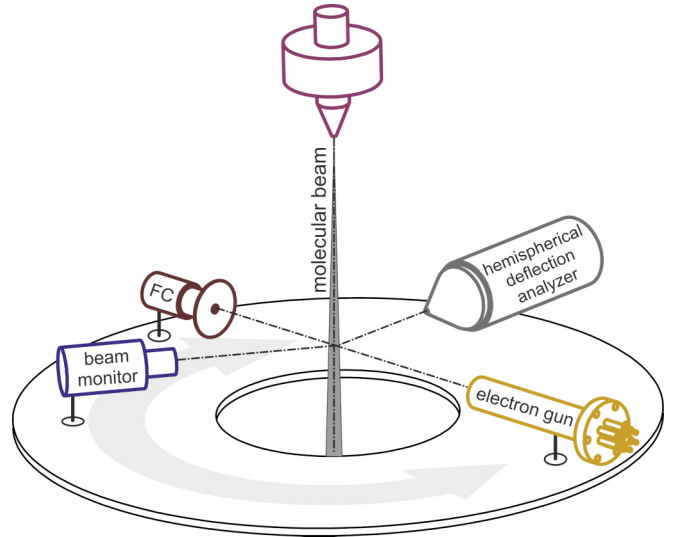


FIG. 1. Schematic view of the present experimental setup. This crossed-beam apparatus, described in detail in a previous paper [13], contains an electron gun, a Faraday cup (FC), and a capillary, all mounted within a vacuum chamber made of μ metal. The entire assembly can be rotated with respect to a hemispherical electron energy analyzer.

generated by an effusion nozzle connected to a gas reservoir, with the reservoir pressure monitored via a capacitance manometer. To track fluctuations in the molecular flow rate, the resulting pressure increase in the vacuum chamber was measured using an ionization gauge. The typical chamber pressure was approximately 2×10^{-5} mbar with the molecular beam and 2×10^{-7} mbar without it.

Scattered primary electrons or, in the case of ionization, ejected secondary electrons are detected by a hemispherical electron energy analyzer using channeltrons as detectors, which records count rates $\frac{\Delta N}{\Delta \Omega \Delta E}$ as a function of secondary electron energy E per energy bin ΔE and per solid angle $\Delta \Omega$. The energy resolution of the electron energy analyzers in both setups was approximately 1.7 eV at a primary energy of $T = 1$ keV and better than 0.7 eV for energies below 100 eV. It is worth noting that these resolutions were insufficient to resolve vibrational and rotational excitations from elastic scattering. The detection angle is varied either by rotating the analyzer (in the first setup) or by rotating the electron gun (in the second setup), with an angular resolution of approximately 1.5° .

One of the main challenges in measuring differential cross sections using a crossed-beam arrangement is accurately determining the interaction volume between the electron and molecular beam, as well as accounting for variations in the solid angle viewed by the electron energy analyzer across this volume. To overcome these difficulties, the relative flow technique (RFT) [15,16] is usually employed. In this method, the electron emission spectra $\frac{\Delta N}{\Delta \Omega \Delta E}$ of both the gas of interest and a reference gas are measured under identical operational conditions of the electron gun, ensuring an identical electron beam profile. It is generally assumed that molecular beams from the same nozzle have identical angular profiles if their intermolecular mean free paths are equal. To satisfy this condition, the gas densities are adjusted to be inversely

proportional to the squares of the kinetic diameters of the respective molecules. Although the relative flow technique accounts for the variation in the detection solid angle across the interaction volume, the entrance aperture and the electrooptical parameters of the electron energy analyzer were configured so that the detection solid angle remained nearly constant over the range of scattering or emission angles studied in the present work. This constancy was verified by comparing the measured positions of resonance-like minima in the DCSs of argon at various incident energies with their well-established theoretical values. In this work, nitrogen was used as the reference gas. The cross sections of nitrogen (see Appendix B) were previously measured in an independent experiment using a different methodology [17]. The differential cross section for a given primary energy T can be obtained by

$$\left(\frac{d^2\sigma}{d\Omega dE}\right)_1 / \left(\frac{d^2\sigma}{d\Omega dE}\right)_2 = \left[\left(\frac{\Delta\dot{N}}{\Delta\Omega\Delta E}\right)_1 / \left(\frac{\Delta\dot{N}}{\Delta\Omega\Delta E}\right)_2 \right] \frac{I_2}{I_1} \sqrt{\frac{M_2}{M_1}} \frac{Z_{\text{flow}2}}{Z_{\text{flow}1}}, \quad (1)$$

where subscripts 1 and 2 refer to the target and reference molecule, respectively, M is the molecular mass, and Z_{flow} is the particle flow rate through the gas nozzle. In the case of differential elastic scattering, $\frac{d^2\sigma}{d\Omega dE}$ and $\frac{\Delta\dot{N}}{\Delta\Omega\Delta E}$ in Eq. (1) must be replaced by $\frac{d\sigma}{d\Omega}$ and $\frac{\Delta\dot{N}}{\Delta\Omega}$, respectively.

The driving pressures over the gas nozzle were adjusted such that the gas effusion occurred within the Clausing flow regime, characterized by Knudsen numbers $Kn_d > 1$. In this work, the Knudsen numbers, calculated based on gas kinetic diameters of 0.364 nm for NH_3 [18] and 0.364 nm for N_2 [19], range between 1.8 and 3.4. Furthermore, the selected driving pressure represented a suitable compromise, ensuring the single collision condition was met while also providing sufficient count rates to maintain statistical uncertainties in the electron energy spectra below 5%.

Notably, our own reference DCS data of N_2 were not available for scattering angles below 20° . Although low-angle measurements have been reported in the literature, such as those reported by Dubois and Rudd [20] and Shyn and Carignan [21], the available data do not cover all combinations of scattering angle and incident electron energy relevant to the present work. Furthermore, these datasets were obtained using different experimental setups, normalization procedures, and reference data, which can introduce systematic differences. For the sake of methodological consistency across all scattering angles and electron energies, we exclusively used our own reference data for $\theta_s \geq 30^\circ$. For smaller scattering angles ($\theta_s \leq 30^\circ$), we assumed that the interaction volume and detection solid angle remain essentially unchanged. Under this assumption, the DCS values were determined using the ratio of the DCS of NH_3 to the elastic count rate (normalized to the electron beam current and gas density) at 30° as the reference. The DCSs at $\theta_s < 30^\circ$ were then obtained by multiplying this ratio by the corresponding normalized elastic count rates. This procedure introduced larger uncertainties at lower scattering angles. These uncertainties were estimated from the mean discrepancy between DCSs at $\theta_s > 30^\circ$ determined using the RFT with nitrogen reference data and those

TABLE I. Molecular geometry and polarizability of NH_3 determined through Hartree-Fock optimization using the GAUSSIAN09 software. The atomic coordinates x , y , and z are given in units of Å and the polarizability tensor elements α_{ij} are provided in atomic units.

	x	y	z	α	
N	0.000000	0.000000	0.109829	$\alpha_{xx} = \alpha_{yy}$	7.928
H	0.000000	0.931698	-0.256268	α_{zz}	2.841
H	-0.806874	-0.465849	-0.256268	$\alpha_{xz} = \alpha_{yz} = \alpha_{xy}$	0.000
H	0.806874	-0.465849	-0.256268		

obtained using the DCS of NH_3 at 30° as the reference, as described above.

The overall uncertainties in the DCS measurements were approximately 16% for scattering angles above 30° , increasing to 20% at scattering angles $\theta_s < 30^\circ$. The uncertainties associated with the DDCS measurements were estimated to be around 25%. A detailed discussion of the individual sources of the uncertainty is provided in Refs. [13,14]. As noted above, the present DCSs include contributions from vibrational and rotational excitation cross sections, which leads to larger DCSs than measurements performed with higher energy resolution. Estimations using the software polydcs [22] indicate that these contributions are in the order of the uncertainties (see below).

III. THEORETICAL METHODS

Differential elastic scattering and doubly differential ionization cross sections were calculated using the IAM-SCAR + I method and the DWBA approach. These calculations require the molecular geometry, as well as the static V_{st} , correlation-polarization V_{cp} , and exchange potentials V_{ex} of the target molecule, along with its molecular wave functions and electron densities. The required molecular properties were calculated using the Hartree-Fock method as implemented in the GAUSSIAN09 program suite, employing the 6-311G basis set augmented with (d,p) polarization functions. The outputs of the Hartree-Fock calculations, including the optimized molecular geometry, the orbital binding energies, and mean kinetic energies, are presented in Tables I and II. Notably, the short-range correlation-polarization potential

TABLE II. Calculated orbital binding B and mean kinetic energies U of the molecular orbitals of NH_3 . The energies are given in eV. Additionally, the occupation number n of each orbital as well as the core or valence effective charges $Z_{\text{eff}}^{c,v}$ are provided. The columns B_s and U_s are obtained by rescaling the computed orbital binding energies and mean kinetic energies using the experimental ionization threshold (indicated by an asterisk “*”) [12].

MO	B	B_s	U	U_s	n	Z_{eff}^c	Z_{eff}^v
1a ₁	422.38	376.74	601.86	536.82	2	9	
2a ₁	30.92	27.58	48.68	43.42	2	7	
1e	17.16	15.31	35.59	31.74	4		1
3a ₁	11.29	10.07*	43.28	38.60	2		1

was determined using the modified free-electron gas model [23], based on Hartree-Fock electron densities. For the outermost asymptotic region, the polarization potential was calculated from the polarizability tensors listed in Table I, using the formula given in Ref. [24].

To facilitate theoretical and numerical treatment of electron scattering and ionization, the multicenter potentials, wave functions and electron densities of the molecule, obtained from the GAUSSIAN09 program suite, were expanded around the molecular center of mass using the SCELlib3 library [24]. This single-center expansion enables a straightforward implementation of the DWBA, originally developed for single-center targets such as atoms, into molecular multicenter scattering systems. A comprehensive description of the single-center expansion method can be found in Ref. [23].

A. Elastic scattering

The elastic DCSs were calculated using the independent atom model with screening corrected additivity rule and interference (IAM-SCAR + I) [10,11]. This method is a widely accepted approximation for describing electron scattering from polyatomic molecules at intermediate and high energies.

In its predecessor, the independent atom model with additivity rule (IAM-AR), the molecular DCS is obtained by summing the squared scattering amplitudes $f_i(\theta)$ of each atomic constituent (N, H). The IAM-SCAR + I improves upon this approximation by incorporating interatomic screening and interference effects [10,11]. With these correction terms, the range of the method's validity may extend to lower incident electron energies, potentially down to 20 eV–30 eV [25].

As described in our previous work [14], the elastic DCS was obtained by summing the contributions from the IAM-SCAR + I terms and the molecular polarization effects. The polarization contribution was derived using the correlation-polarization potential of the entire molecule, rather than that of the individual atomic constituents. It is worth noting that the scattering amplitudes of the atomic constituents were obtained using complex phase shifts to account for the attenuation of the incoming electron waves due to inelastic channels. As the exact expression for the calculation of the elastic DCS is provided in Ref. [14], it is not repeated here.

B. Electron-impact ionization

Triply differential cross sections (TDCSs) for electron-impact ionization were computed using the distorted wave Born approximation (DWBA), employing single-center expanded (SCE) molecular potentials, wave functions, and electron densities as mentioned above. As the theoretical methods used in this work are discussed in detail in our previous publication [13], only a brief summary is provided below.

The TDCS for electron ejection from the i th molecular orbital (MO) is given by

$$\frac{d^3\sigma_i}{d\Omega_A d\Omega_B dE_B} = (2\pi)^4 \frac{n_i k_A k_B}{k_0} [|T_{\text{dir}}|^2 + |T_{\text{ex}}|^2 - \text{Re}(T_{\text{dir}}^* T_{\text{ex}})], \quad (2)$$

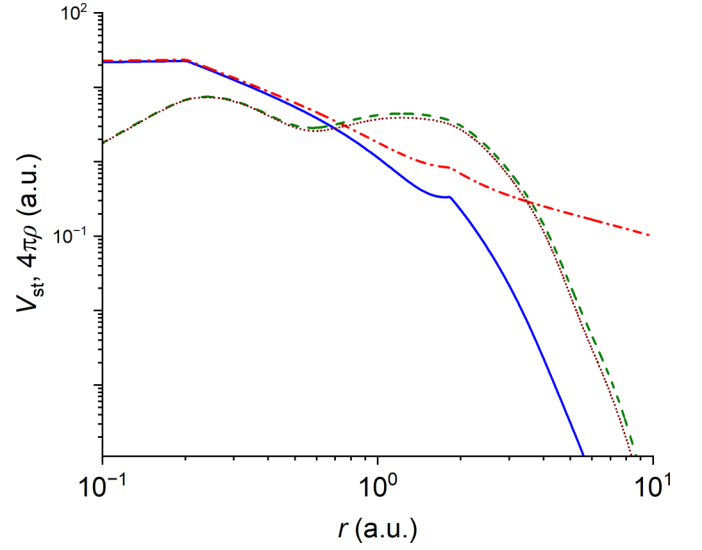


FIG. 2. Static potentials V_{st} and radial electron densities $4\pi\rho$ used for the DWBA calculations in atomic units: V_{st} for NH_3 (blue solid line), V_{st} for NH_3^+ (red dash-dotted line), $4\pi\rho$ for NH_3 (green dashed line), and $4\pi\rho$ for NH_3^+ (brown dotted line).

where n_i is the number of electrons in the orbital, k_0 is the momentum of the incoming electron, and $k_{A,B}$ are the momenta of the scattered and ejected electrons, respectively. The terms T_{dir} and T_{ex} refer to the direct and exchange transition matrix elements. The direct T matrix is defined as

$$T_{\text{dir}}(\mathbf{k}_0, \mathbf{k}_A, \mathbf{k}_B) = \langle \chi^-(\mathbf{k}_A, \mathbf{r}_A) \chi^-(\mathbf{k}_B, \mathbf{r}_B) | V_{\text{ee}} | \psi_i(\mathbf{r}_B) \chi^+(\mathbf{k}_0, \mathbf{r}_A) \rangle, \quad (3)$$

where V_{ee} denotes the electron-electron interaction potential, $\psi_i(\mathbf{r}_B)$ is the wave function of the i th molecular orbital, and $\chi^\pm$ represent the distorted wave functions of the incident and scattered or ejected electrons. The exchange T matrix can be obtained by interchanging the coordinates of the scattered and ejected electrons. The distorted waves are solutions to the one-electron elastic scattering equations

$$(K_0 + U_i) \chi^+ = E_0 \chi^+, \quad (4)$$

$$(K_{A,B} + U_f) \chi_{A,B}^- = E_{A,B} \chi_{A,B}^-, \quad (5)$$

where K denotes the kinetic energy operator, $E_{A,B}$ the kinetic energy of the outgoing electrons, and $E_0 = T$. In the first-order DWBA, the spherically symmetric optical potentials of the neutral target molecule and resulting ion are typically taken as the initial and final distorting potentials, U_i and U_f , respectively. In this work, we adopt the sum of the electrostatic potential V_{st} and the exchange potential as the distorting potentials. Figure 2 presents V_{st} for NH_3 and NH_3^+ , along with the radial electron density employed to compute the exchange potential using the formula of Furness and McCarthy [26].

1. Single center expansion and orientation averaging

For atoms, where wave functions are centered on a single nucleus, the computational form of Eq. (3) can be simplified to

a one-dimensional problem by factorizing the wave functions and Coulomb potential into angular and radial parts using the partial wave expansion method (see. Refs. [13,27]). For molecules, however, such factorization is much more difficult due to their multicenter nature.

In our single-center expansion (SCE) approach, molecular wave functions are expanded about the center of mass using single-center symmetry adapted angular functions

$$\psi_i(\mathbf{r}_B) = \frac{1}{r_B} \sum_{lm} b_{lm}^{p_i} u_{lm}^i(r_B) Y_{lm}(\hat{\mathbf{r}}_B). \quad (6)$$

Here, p_i denotes the irreducible representation (IRREP) of the i th molecular orbital, which can take the values A_1 , A_2 , or E in the case of the ammonia molecule, belonging to the C_{3v} point group. The functions Y_{lm} are spherical harmonics, and the coefficients $b_{lm}^{p_i}$ can be determined from the character tables of the corresponding IRREP. The radial functions u_{lm}^i are obtained using the SCELlib library.

Since the molecules in the gas beam are randomly oriented, the theoretical TDCS must be averaged over all possible molecular orientations to enable direct comparison with experimental data. The orientation of molecular wave functions can be modified using the Wigner D matrix $D_{m'l',m}^l(\alpha, \beta, \gamma)$:

$$\begin{aligned} & \langle \hat{\mathbf{r}}'_B | \hat{R}(\alpha, \beta, \gamma) | \psi_i \rangle \\ &= \frac{1}{r_B} \sum_{lm} b_{lm}^{p_i} u_{lm}^i(r_B) D_{m'l',m}^l(\alpha, \beta, \gamma) Y_{lm'}(\hat{\mathbf{r}}'_B), \end{aligned} \quad (7)$$

where α , β , and γ are the Euler angles.

The orientation-averaged transition matrix element can be obtained by substituting ψ_i in Eq. (6) with the rotated wave function given on the right-hand side in Eq. (7), and subsequently integrating over the Euler angles

$$\overline{|T|^2} = \frac{1}{8\pi^2} \int_0^{2\pi} d\alpha \int_0^\pi d\beta \sin\beta \int_0^{2\pi} d\gamma |T(\alpha, \beta, \gamma)|^2. \quad (8)$$

This method yields more accurate TDCS than the commonly used orientation-averaged molecular orbital (OAMO) approximation, which averages only the molecular wave function ψ_i instead of the full transition matrix element.

2. Postcollision interaction

Postcollision interactions (PCI) can be incorporated into the TDCS by inserting a correction factor $C_{e,-e}$ between the distorted wave functions of the scattered and ejected electrons in the bra vector of Eq. (3). In this work, we employ the correction factor expression proposed by Ward and Macek [28]

$$|C_{e,-e}|^2 = \left| e^{-\frac{\pi\gamma}{2}} \Gamma(1 - i\gamma) {}_1F_1(i\gamma, 1, -2ik_{AB}r_{AB}^{av}) \right|^2, \quad (9)$$

where $\Gamma(1 - i\gamma)$ is a gamma factor, ${}_1F_1$ is a confluent hypergeometric function, $k_{AB} = \frac{1}{2}|\mathbf{k}_A - \mathbf{k}_B|$, and $\gamma = 1/2k_{AB}$ is the Sommerfeld parameter. The average electron-electron distance r_{AB}^{av} is approximated as a function of the total energy $E_t = E_A + E_B$ of the outgoing electrons

$$r_{AB}^{av} = \frac{\pi^2}{16E_t} \left(1 + \frac{0.627}{\pi} \sqrt{E_t} \ln E_t \right)^2. \quad (10)$$

Under this approximation, the PCI factor $C_{e,-e}$ becomes independent of the radial coordinates of the interacting electrons, allowing it to be factored out of the bra vector in Eq. (3). Consequently, the PCI can be simply accounted for by multiplying the T matrix with $C_{e,-e}$:

$$\overline{|T_{\text{PCI}}|^2} = |C_{e,-e}|^2 \times \overline{|T|^2}. \quad (11)$$

In our earlier study on pyrimidine [13], the doubly differential cross section (DDCS) was obtained through analytical integration of the TDCS

$$\frac{d^2\sigma_{\text{dir}}}{d\Omega_B dE_B} = (2\pi)^4 \frac{n_i k_A k_B}{k_0} \int d\Omega_A \overline{|T_{\text{dir}}|^2} \quad (12a)$$

$$= \frac{4n_i}{k_0^3 k_A k_B} \sum_{lm} \int d\Omega_A \left| \sum_{L'M'} a_{lmL'M'} Y_{L'M'}(\Omega_A) \right|^2, \quad (12b)$$

by exploiting the orthogonality of spherical harmonics. However, the inclusion of the angle-dependent PCI factor $|C_{e,-e}(|\mathbf{k}_A - \mathbf{k}_B|)|^2$ in the TDCS complicates the integration, making an analytical approach impractical. Therefore, the theoretical DDCS presented below were obtained via numerical integration of the TDCS including PCI effects [Eq. (11)].

C. Generalized binary encounter Bethe model

The binary encounter Bethe model (BEB) [29] is a well-established method for calculating the total (TICS) and singly differential ionization cross sections (SDCS) of molecules. The total ionization cross section σ is given by

$$\sigma = \sum_i \frac{S_i}{t_i + (u_i + 1)/v_i} \left[\frac{\ln t_i}{2} \left(1 - \frac{1}{t_i^2} \right) + 1 - \frac{1}{t_i} - \frac{\ln t_i}{t_i + 1} \right], \quad (13)$$

where the scaling factor is defined as $S = 4\pi a_0^2 n_i (R/B_i)^2$, with a_0 being the Bohr radius, R the Rydberg constant, n_i the occupation number of the i th molecular orbital, $t_i = T/B_i$, $u_i = U_i/B_i$, and v_i a correction factor. The SDCS can be calculated using the expression

$$\begin{aligned} \frac{d\sigma}{d\epsilon}(\epsilon, t) &= \sum_i \frac{S_i}{t_i + (u_i + 1)/v_i} \\ &\times \sum_{k=1}^3 F_k(t_i) [(\epsilon_i + 1)^{-k} + (t_i - \epsilon_i)^{-k}], \end{aligned} \quad (14)$$

where

$$F_1 = -(t_i + 1)^{-1}, \quad F_2 = 1, \quad F_3 = \ln(t_i). \quad (15)$$

The BEB model simplifies calculations, as it only requires the occupation number n_i , kinetic energy U_i , and binding energy B_i of each molecular orbital. The correction factor v_i was introduced to improve agreement between theoretical predictions and experimental data. Physically, the correction factor reduces the overestimation of the kinetic energy gain of the incident electron from the released electron's potential

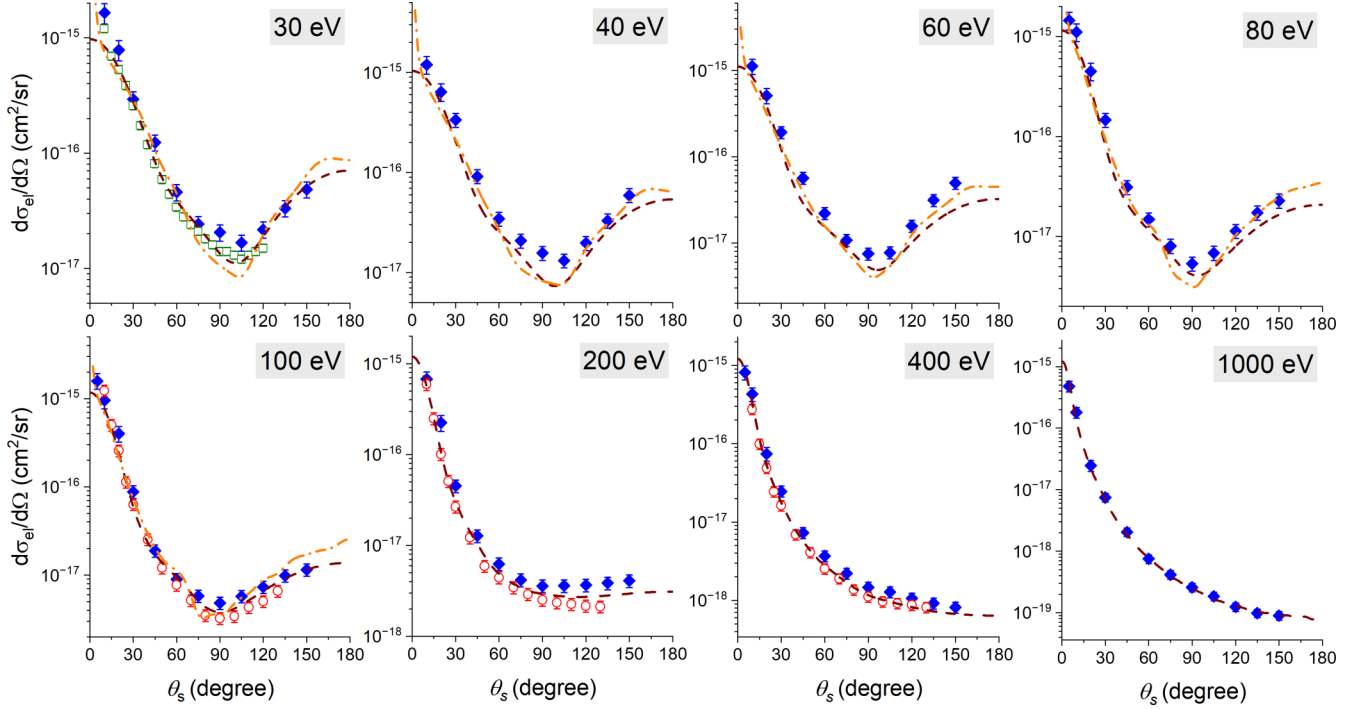


FIG. 3. Elastic DCS of NH_3 for different electron energies T . The present experimental results ($\blacklozenge$) are compared to experimental data of Homem *et al.* [5] ($\circ$), and Alle *et al.* [4] ($\square$). Additionally, calculations using the IAM-SCAR + I (brown dashed lines) and polydcs code (orange dash dotted lines) are depicted.

energy by accounting for the attractive force exerted by the ionized target molecule on the incident electron.

A recent development is the generalized BEB model with acceleration correction (GBEB) proposed by Wang *et al.* [30] in which the variation in kinetic energy is estimated based on Gauss' law. In this model, the correction factor is defined in terms of $Z_{\text{eff}}^{c,v}$, the molecular effective charge experienced by the incident electron. The value of $Z_{\text{eff}}^{c,v}$ depends on the MO from which the electron is ejected, particularly on whether the MO is a core or valence orbital. The procedure for determining the effective charges is detailed in Ref. [30], and the corresponding values are listed in Table II.

Finally, molecular orbital binding energies obtained from quantum chemistry calculations often overestimate the effective energy required for ionization from the corresponding orbital. To address this, Champion *et al.* [31] applied a scaling procedure that adjusts both the binding energies and the mean kinetic energies based on the discrepancy between the theoretical and experimental ionization thresholds. An additional calculation of the TICS is performed in this work using the BEB model with the scaling procedure proposed by Champion *et al.* [31] (see Table II).

IV. RESULTS AND DISCUSSION

All experimental results are presented in tabular form in Appendix A.

A. Elastic cross sections

1. Singly differential elastic cross sections

Figure 3 compares the DCSs of NH_3 measured in this work (see Table III) with both existing literature data and theoretical predictions from the IAM-SCAR + I model and the polydcs code. At 1 keV, the present results show excellent agreement with the IAM-SCAR + I calculations, which primarily represent the summed DCSs of the atomic constituents at high energies. At 400 eV, the agreement between experimental and theoretical results is relatively good; however, the present data exceed those reported by Homem *et al.* [5] by approximately 30%. The discrepancy becomes more pronounced at 200 eV, where the present results are up to 70% higher than Homem *et al.*'s [5] values, indicating possible systematic differences in the experimental methodologies. Since both studies employed the RFT, these differences may originate from systematic factors such as the choice of reference datasets and the method of flow rate determination. Notably, the IAM-SCAR + I predictions lie approximately midway between the two datasets. At 100 eV, the agreement between the current measurements and the IAM-SCAR + I model remains good, with the theoretical results closely reproducing the observed trends. At scattering angles below 10° , noticeable differences were observed between the experimental data and IAM-SCAR + I calculations, whereas the polydcs code, which incorporates rotational excitations, reproduces the experimental values well in this angular region. This underscores significance of rotational excitations in low-angle scattering.

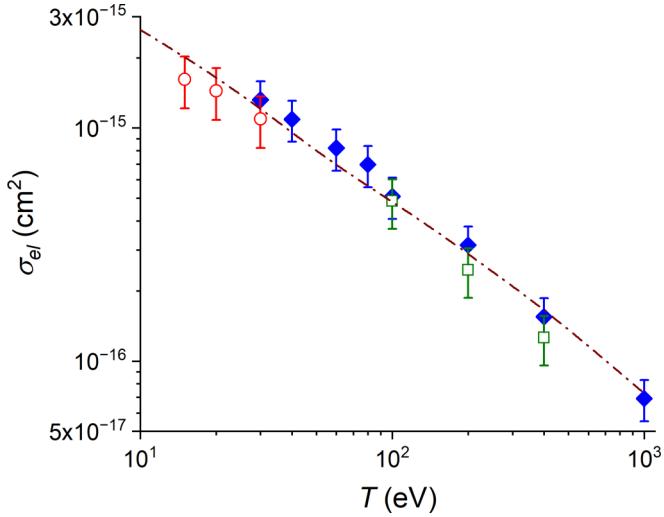


FIG. 4. TECS of NH_3 . The present experimental results ($\blacklozenge$) are compared to experimental data from Homem *et al.* [5] ($\square$), Alle *et al.* [4] ($\circ$), as well as theoretical values calculated using the volscat code [32] (dashed line).

At 80 eV, the present experimental data remain in good agreement with the IAM-SCAR + I model and qualitatively follow the polydcs predictions, although the latter displays a dip near 90° that is not reflected in the measurements. At 60 eV, the experimental DCS values are significantly higher than those predicted by IAM-SCAR + I. The polydcs calculations show better overall agreement, except near 90° , where a pronounced theoretical minimum is again absent in the experimental data. This trend continues at 40 eV, with the present DCSs deviating substantially from both models, particularly around 90° . At the lowest studied energy, 30 eV, agreement with IAM-SCAR + I improves somewhat unexpectedly. However, deviations near 90° persist, reinforcing the consistent pattern of theoretical underestimation in this angular region for energies below 100 eV. Additionally, the present experimental results at 30 eV lie consistently above those of Alle *et al.* [4], which are in good agreement with the IAM-SCAR + I model.

Considering the high-energy resolution of 60 meV for the data reported by Alle *et al.* [4] as well as the good agreement with the IAM-SCAR + I, the systematic shift between both our results and those of Alle *et al.* [4] can be attributed to the unresolved excitation contributions in our experiment. For comparison with Homem *et al.* [5], however, this argument does not apply since their energy resolution is similar to ours. The origin of the difference with their results is therefore likely methodological rather than physical.

The present experimental results demonstrate overall consistency with existing theoretical models, particularly IAM-SCAR + I, at energies above 100 eV. Below this energy, however, the DCSs reveal notable discrepancies, especially near 90° scattering angles. Comparisons with polydcs calculations suggest that rotational effects are crucial for small-angle scattering, especially at low electron energies. The large deviations observed between the present measurements and theoretical predictions at low electron energies reflect the difficulty of accurately modeling electron scattering in this

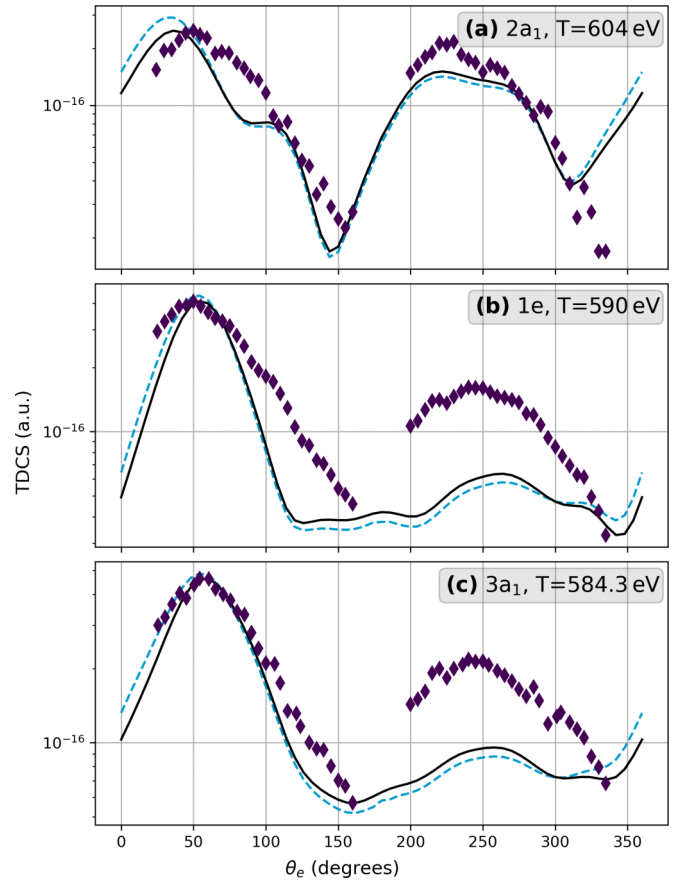


FIG. 5. Theoretical triply differential cross sections (TDCS) calculated using the DWBA with (solid lines) and without (dashed lines) PCI compared to the experimental data of El Mir *et al.* [6] ($\blacklozenge$). The results correspond to an ejected electron energy of 74 eV, with the scattered electron fixed at an energy of 500 eV and a scattering angle of $\theta_s = -6^\circ$. All measurements and calculations were performed in the coplanar asymmetric geometry. The experimental data were normalized to the binary peak of the DWBA-PCI calculations. Panels (a)–(c) correspond to ionization from the valence orbitals: (a) $2a_1$, (b) $1e$, and (c) $3a_1$, respectively.

regime, where multiple scattering mechanisms can play a significant role.

2. Total elastic scattering cross sections

The TECS of NH_3 were determined by integrating the measured DCS over the scattering angle θ_s . Since direct measurements outside the range $10^\circ \leq \theta_s \leq 150^\circ$ were not feasible, the DCS values in these regions ($\theta_s < 10^\circ$ and $\theta_s > 150^\circ$) were obtained through extrapolation of the experimental data. This extrapolation was carried out by fitting a series of Legendre polynomials to the measured DCS values. The resulting DCSs were also employed to calculate the momentum transfer cross sections, with uncertainties amounting to 20% for the TECS and MTCS. Figure 4 shows the present results for the TECS compared with the data reported by Alle *et al.* [4], Homem *et al.* [5], and with theoretical values calculated using the volscat software [32]. Although the present results overlap with those of other authors within the experimental uncertainties, they tend to be systematically higher

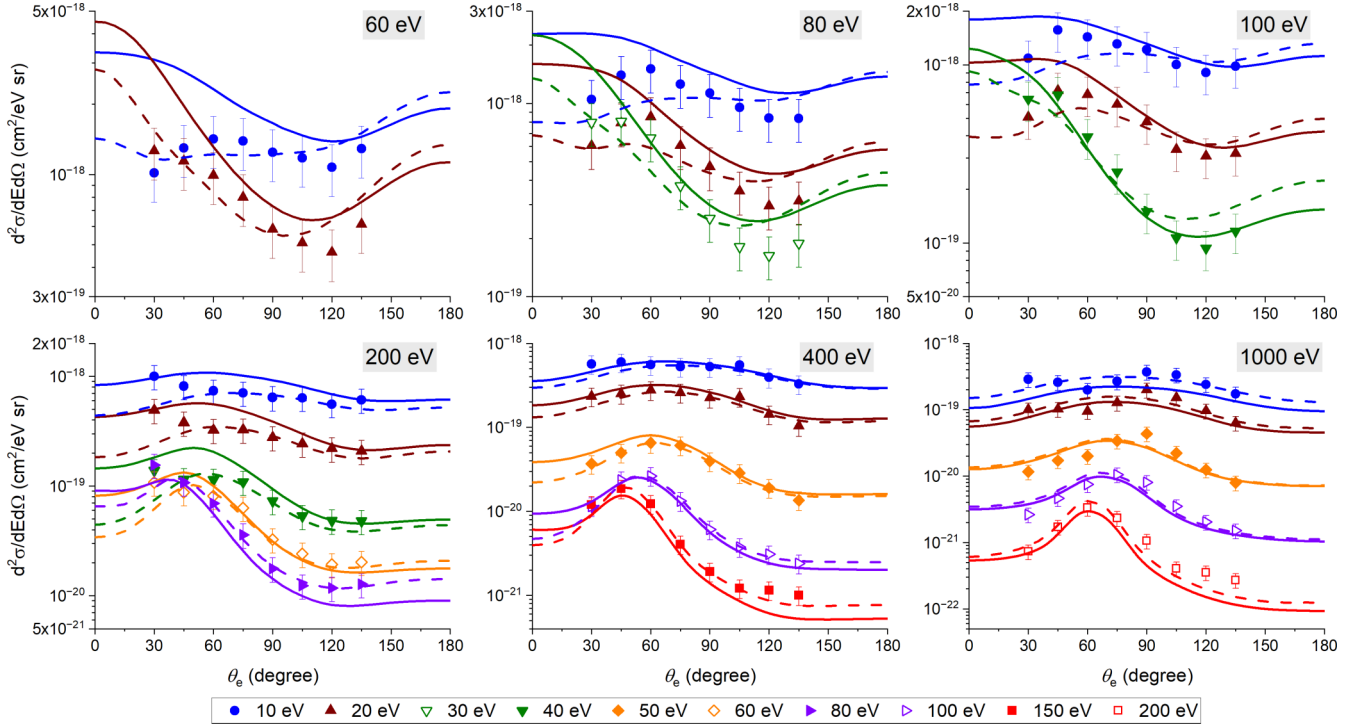


FIG. 6. Doubly differential ionization cross sections of NH_3 as a function of the electron emission angle θ_e at various secondary electron energies E . Experimental results are shown by various markers as indicated in the figure legend and DWBA calculations are shown in their corresponding color with (dashed lines) and without PCI effects (solid lines). The primary energies are indicated in the figure legends.

than the literature data. In comparison with the theoretical values, the data of this work are noticeably higher, particularly at electron energies below 400 eV.

B. Ionization cross sections

1. Triply differential ionization cross sections

In Fig. 5, the experimental angular distribution of 74 eV electrons ejected from NH_3 determined by El Mir *et al.* [6] are compared with the theoretical predictions obtained in the present study. Both the experimental and theoretical results refer to coplanar asymmetric kinematics, with the scattering angle of the primary electron fixed at 6° , and the energy of the scattered electron set to 500 eV. Figures 5(a), 5(b), and 5(c) illustrate ionization from the $2a_1$, $1e$, and $3a_1$ orbitals, respectively, corresponding to incident electron energies of 584.3 eV, 590.6 eV, and 604 eV. While noticeable discrepancies between experiment and theory are evident in the details, the overall shape of the angular distribution, characterized by two peaks in the binary ($0^\circ \leq \theta_e \leq 180^\circ$) and recoil ($180^\circ < \theta_e \leq 360^\circ$) region, is reasonably well captured by the DWBA calculations. These discrepancies become more pronounced for outer-valence orbitals in the recoil region, where the theoretical model tends to significantly underestimate the experimental peak intensities. It is worth noting, however, that accurately modeling of recoil peaks is challenging, as the electrons contributing to these features undergo complex interactions with the molecular potential [33–35]. These interactions are not adequately accounted for in the DWBA based on the first Born approximation.

The best agreement between the experiment and theory is observed for the binary peak associated with the highest occupied molecular orbital (HOMO) $3a_1$, which is primarily composed of the nitrogen atom p orbitals. As shown in Fig. 5(c), both the position and the width of the binary peak are well reproduced by the DWBA calculation. For the recoil peak originating from the $3a_1$ orbital, the experimental position and width also show good agreement with the theoretical predictions. However, the experimental intensity is significantly higher than that predicted by theory. A similar trend is observed for the HOMO-1 orbital $1e$ [see Fig. 5(b)], which also has p -like character. In the difference to the $3a_1$ orbital, the theoretical positions of both the binary and recoil peaks for the $1e$ orbital are slightly higher than the experimental values, and the theoretical peak widths are noticeably narrower than those observed experimentally.

For the innermost valence orbital $2a_1$ [see Fig. 5(a)], theoretical calculations successfully reproduce the experimentally observed increase in recoil peak intensity. The DWBA calculations clearly reveal a shoulder structure at emission angles around 105° and 260° , which is faintly suggested by the experimental data as well. This shoulder is unlikely to originate from a double peak, which typically arises from p -type orbitals with nodal structures, whereas the $2a_1$ orbital is a nonbonding s -type orbital localized on the nitrogen atom. Instead, the shoulder is attributed to a specific kinematic configuration, a conclusion supported by its disappearance when the primary electron scattering angle is slightly increased by 10° .

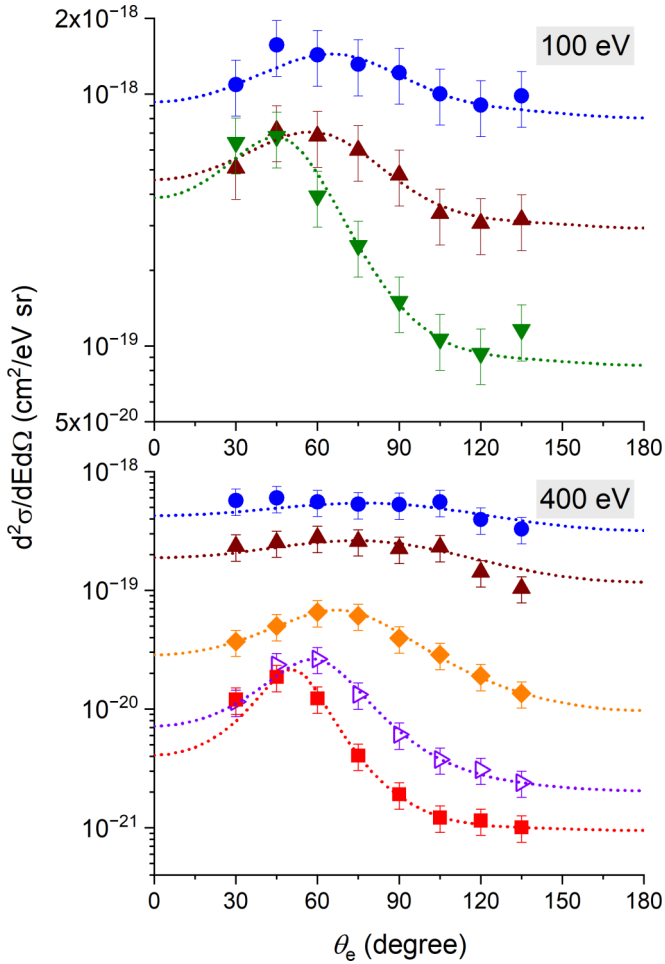


FIG. 7. Examples of the best fits of Eq. (16) to the experimental DDCS are presented for primary energies $T = 100$ eV and $T = 400$ eV. The secondary energies are the same as those shown in Fig. 6.

2. Doubly differential ionization cross sections

Figure 6 presents current experimental and theoretical DDCS of NH_3 as functions of the electron emission angle θ_e for various secondary electron energies E . The DWBA calculations (solid lines) show good agreement with the present experimental data at primary electron energies of 400 eV and 1 keV. However, as the primary electron energy T decreases, the discrepancy between experimental and theoretical results increases. This growing deviation at lower electron energies may be attributed, on one hand, to the reduced validity of the DWBA in this energy regime, and on the other hand, to the increasing influence of additional interactions such as PCI, which become more pronounced at lower electron energies.

To investigate the influence of the PCI on the angular distribution of emitted electrons, the TDCSs were calculated with PCI included. These cross sections were then numerically integrated over the scattering angle of the primary scattered electrons to obtain the DDCS versus the emission angle of secondary electrons. Theoretical angular distributions that include PCI are represented by dashed lines in Fig. 6. As evident from the figure, the DWBA calculations with PCI reproduce the experimental angular distributions reasonably well, also

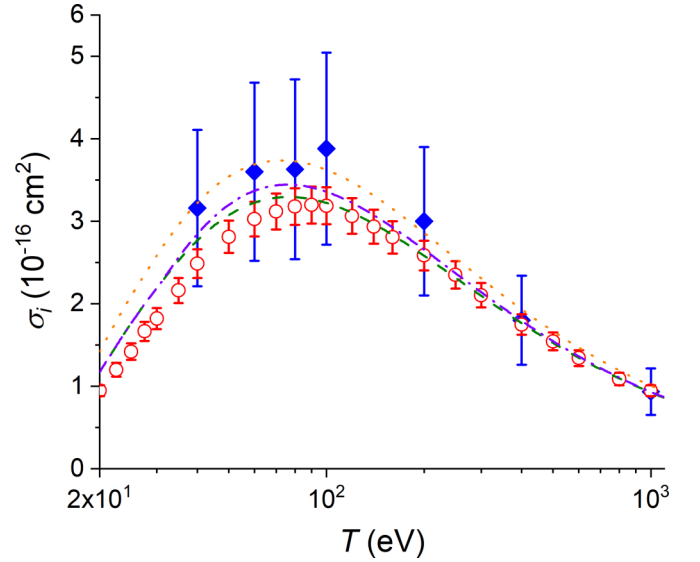


FIG. 8. Total ionization cross sections (TICS) of NH_3 . The present experimental results ($\blacklozenge$) are compared to the experimental data of Rejoub *et al.* [8] ($\circ$), and theoretical calculations: BEB (green dashed line), BEB with scaled orbital binding energies and mean kinetic energies, as proposed by Champion *et al.* [31] (orange dotted line), and GBEB (purple dash-dotted line) models.

at electron energies below 400 eV. As expected, the emission of low-energy secondary electrons occurs rather isotropically while the binary peaks become more pronounced with the increasing secondary electron energy E .

3. Total and singly differential ionization cross sections

The SDCS, $d\sigma_i/dE$, of NH_3 were obtained by integrating the experimental DDCS, $d^2\sigma_i/dEd\Omega$, over the electron emission angle. The DDCS values for the angular ranges $0^\circ \leq \theta_e < 30^\circ$ and $135^\circ < \theta_e \leq 180^\circ$ were estimated through extrapolation of the measured data. For this purpose, the experimental values within the measured angular range were fitted using a semiempirical formula comprising two Lorentzian functions, which has been shown to reasonably represent molecular DDCS [36,37]

$$\frac{d\sigma_i^2}{dEd\theta_e} = A_1[f_{\text{BE}}(\varepsilon, t, \theta_e) + A_2f_{\text{b}}(\varepsilon, t, \theta_e)], \quad (16)$$

with dimensionless variables $t = T/I$, $\varepsilon = E/I$, where I is the ionization energy of NH_3 , and A_1 and A_2 are fit parameters. Figure 7 illustrates representative best fits of Eq. (16) to the experimental data for primary electron energies of 100 eV and 400 eV. Figure 7 demonstrates that the DDCS can be effectively modeled by a combination of two Lorentzian functions, representing the binary encounter peak and the backward emission. Similar agreement was observed at other primary electron energies as well. The SDCS obtained in this way was subsequently integrated over the secondary electron energy E to determine the TICS σ_i . It should be noted that the SDCS below 5 eV was estimated by extrapolating the SDCS to lower secondary electron energies based on the energy dependence predicted by the DWBA.

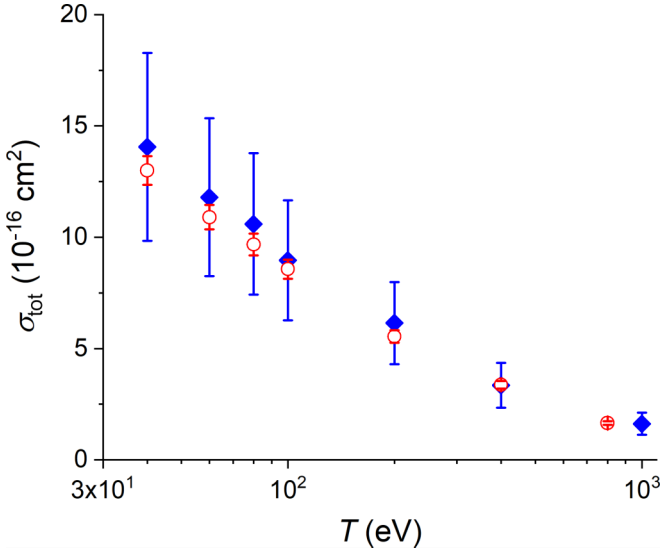


FIG. 9. Total electron scattering cross sections of NH_3 , obtained by summing the experimental total elastic and ionization cross sections ($\blacklozenge$). For comparison, the experimental values compiled by Itikawa [2] ($\circ$) are also shown.

In Fig. 8, the TICS obtained from the present measurements are compared with the data reported by Rejoub *et al.* [8], who determined the TICS by measuring the count rates of fragment and parent ions following electron impact. The two datasets agree within the experimental uncertainties, although the present results are systematically higher than those of Rejoub *et al.* [8]. This overestimation may stem from inaccuracies in extrapolating the present experimental data beyond the measured emission angles, as well as to secondary electron energies below 5 eV. A similar trend is observed when comparing with theoretical predictions from the BEB model. However, excellent agreement is observed between the present experimental results and BEB model predictions,

when using rescaled orbital binding energies and mean kinetic energies [31].

C. Total scattering cross section

Figure 9 compares the sum of the TICS and TECS determined in this work with the recommended total electron scattering cross sections of NH_3 [2]. This comparison is appropriate, as the contribution of discrete excitation cross sections of NH_3 to the TCS in the measured energy range is expected to be smaller than the associated uncertainties. For $T \geq 100$ eV, the present results agree well with the total electron scattering cross sections recommended by Itikawa [2] within the experimental uncertainties, supporting the consistency of the measured elastic scattering and ionization cross sections.

V. CONCLUSION

The differential elastic scattering cross sections of NH_3 measured in this work tend to be higher than those reported in the literature [4,5]. This systematic increase is mainly attributed to contributions from unresolved rotational and vibrational excitation channels, as well as possible systematic differences in the application of the relative flow technique. Nevertheless, the deviations are generally modest, extending only slightly beyond the experimental uncertainties. Overall, the experimental results show reasonably good agreement with theoretical predictions from both the IAM-SCAR + I model and the polydcs code, except at scattering angles around 90° , where pronounced minima are observed for $T \leq 100$ eV. In this region, the theoretical values are significantly lower than the present experimental results. The polydcs code, which accounts for rotational excitations, shows improved agreement at low scattering angles. The total elastic scattering cross sections of NH_3 , obtained by integrating the DCS over

TABLE III. Experimental differential elastic scattering cross sections (DCS) of NH_3 for different primary energies T and scattering angles θ_s . The DCS are given in units of $10^{-18} \text{ cm}^2/\text{sr}$ with an overall uncertainty of 16% for $\theta_s \geq 30^\circ$. The TECS and MTCS are given in units of 10^{-16} cm^2 with an overall uncertainty of 20%. Numbers in italics (below 30°) are the DCSs estimated using the DCS of NH_3 at $\theta_s = 30^\circ$ as the reference. These have a higher uncertainty of approximately 20%.

θ_s/T	30 eV	40 eV	60 eV	80 eV	100 eV	200 eV	400 eV	1000 eV
5°	—	—	—	1442	1585	—	811	479
10°	1645	1200	1120	1103	952	675	428	180
20°	784	638	510	448	400	224	74	25
30°	292	335	192	146	88	45	25	7.45
45°	123	92	57	31	18.9	12.7	7.26	2.05
60°	46	34	22	14.8	8.95	6.24	3.67	0.75
75°	24	21	10.8	8.03	5.78	4.16	2.21	0.41
90°	20	15.6	7.49	5.34	4.83	3.59	1.47	0.26
105°	16.7	13.2	7.74	6.84	5.74	3.59	1.28	0.18
120°	22	20	15.8	11.3	7.35	3.66	1.05	0.12
135°	33	33	31	17.3	9.8	3.85	0.91	0.10
150°	48	59	50	23	11.5	4.08	0.81	0.09
TECS	13.2	10.9	8.2	7.0	5.09	3.15	1.55	0.69
MTCS	4.7	4.5	3.3	2.0	1.24	0.63	0.24	0.051

TABLE IV. Present experimental doubly differential ionization cross sections of NH_3 . The DDCSs are given in units of $10^{-20} \text{ cm}^2 \text{ eV}^{-1} \text{ sr}^{-1}$. Experimental uncertainties amount to 25%.

$T = 60 \text{ eV}$		DDCS						
$E \text{ (eV)}$	30°	45°	60°	75°	90°	105°	120°	135°
5	146	176	219	212	205	222	193	224
10	102	130	142	139	124	117	107	129
20	126	114	99	80	58	51	46	61
$T = 80 \text{ eV}$		DDCS						
$E \text{ (eV)}$	30°	45°	60°	75°	90°	105°	120°	135°
5	226	224	237	199	192	176	159	165
10	105	140	151	126	113	95	84	84
20	60	79	85	60	47.0	35.1	29.4	31.3
30	80	81	66	37.5	25.4	18.1	16.3	18.9
$T = 100 \text{ eV}$		DDCS						
$E \text{ (eV)}$	30°	45°	60°	75°	90°	105°	120°	135°
5	166	239	228	201	209	187	189	189
10	109	157	143	131	121	100	90	98
20	50.9	72	68	60	47.8	33.6	30.7	31.8
40	64	68	39.4	25.0	15.0	10.7	9.3	11.6
$T = 200 \text{ eV}$		DDCS						
$E \text{ (eV)}$	30°	45°	60°	75°	90°	105°	120°	135°
5	175	153	147	121	112	114	110	117
10	100	81	74	71	64	64	56	61
20	49.2	37.8	32.3	32.9	27.7	24.3	22.0	20.8
40	13.9	11.5	11.4	10.9	7.3	5.3	4.8	4.8
60	10.8	8.8	8.1	6.3	3.3	2.4	1.9	2.0
80	15.6	10.8	6.9	3.6	1.8	1.24	1.18	1.27
$T = 400 \text{ eV}$		DDCS						
$E \text{ (eV)}$	30°	45°	60°	75°	90°	105°	120°	135°
5	101	107	103	95	90	100	85	64
10	57	60	55	52.9	52.6	55.4	39.4	32.8
20	23.4	25.2	27.8	25.9	22.4	23.2	14.3	10.4
50	3.7	5.0	6.5	6.1	4.0	2.9	1.9	1.4
100	1.15	2.4	2.6	1.3	0.61	0.38	0.31	0.24
150	1.20	1.9	1.22	0.40	0.19	0.122	0.115	0.101
$T = 1 \text{ keV}$		DDCS						
$E \text{ (eV)}$	30°	45°	60°	75°	90°	105°	120°	135°
5	61	56	40.7	56	85	69	54.0	33.6
10	28.6	25.9	19.8	26.6	37.1	33.5	24.0	17.4
20	10.0	10.2	9.4	12.7	19.9	15.1	9.6	6.3
50	1.16	1.7	2.0	3.4	4.3	2.2	1.24	0.80
100	0.26	0.46	0.75	1.05	0.81	0.35	0.20	0.15
200	0.073	0.17	0.33	0.23	0.106	0.040	0.035	0.027
300	0.045	0.144	0.18	0.058	0.032	0.013	0.0112	0.0094
400	0.068	0.175	0.077	0.022	0.016	0.0074	0.0071	0.0058

the scattering angle exhibits good agreement with the predictions of the volscat code within the experimental uncertainties.

The accuracy of the DWBA was evaluated using the TDCS of NH_3 measured by El Mir *et al.* [6] under coplanar asymmetric kinematics at incident electron energies around 600 eV.

TABLE V. Singly differential ionization cross sections of NH_3 in units of $10^{-18} \text{ cm}^2 \text{ eV}^{-1}$ obtained by integrating the experimental DDCSs over the emission angle (Table IV). The TICSs, determined by integrating the SDCSs over the secondary electron energies, are presented in units of 10^{-18} cm^2 . Primary T and secondary electron energies E are given in eV. The uncertainties amounted to approximately 28% for the SDCS, and 30% for the TICSs.

E/T	60	80	100	200	400	1000
4	30	27	28	20	14	9.2
5	26	24	25	18	11.6	7.4
6	23	21	22	16	10.9	6.0
7	21	19	19	13	8.3	4.88
8	19	17	18	11.8	7.5	4.13
9	18	15	16	10.6	6.8	3.51
10	16	14	14	9.7	5.92	3.15
12	14	11.0	11.6	8.0	5.03	2.66
14	12.0	9.7	9.7	7.0	4.40	2.19
16	10.7	8.5	8.0	5.89	3.88	1.810
18	9.6	7.4	6.9	4.89	3.46	1.550
20	8.9	6.3	5.93	4.03	2.64	1.310
25	—	5.05	4.27	2.63	1.610	0.893
30	—	4.73	3.64	1.930	1.210	0.624
35	—	—	3.33	1.470	0.885	0.467
40	—	—	3.29	1.160	0.676	0.440
50	—	—	—	0.814	0.469	0.239
60	—	—	—	0.689	0.329	0.167
70	—	—	—	0.606	0.247	0.121
80	—	—	—	0.587	0.198	0.091
90	—	—	—	0.595	0.149	0.073
100	—	—	—	—	0.122	0.058
120	—	—	—	—	0.094	0.042
140	—	—	—	—	0.076	0.029
160	—	—	—	—	0.061	0.022
180	—	—	—	—	0.055	0.017
200	—	—	—	—	—	0.014
300	—	—	—	—	—	0.006
350	—	—	—	—	—	0.005
400	—	—	—	—	—	0.005
450	—	—	—	—	—	0.004
TICS	360	363	388	300	180	94

While the DWBA calculations successfully reproduce the general features of the angular distribution of secondary electrons, notable discrepancies were observed in the ratio of the binary to recoil peak heights. Nevertheless, remarkably good agreement was achieved between the experimental DDCS and the DWBA calculations for incident electron energies as low as 60 eV when postcollision interactions were taken into account.

Total ionization cross sections (TICS), obtained by integrating the measured DDCS over emission angle and secondary electron energy, agree with the experimental results of Rejoub *et al.* [8] within the experimental uncertainties. However, the present results tend to be slightly higher than the data of Rejoub *et al.* [8] at electron energies below 200 eV, which may be due to uncertainties associated with extrapolating the present experimental data beyond measured angular and energy ranges. When compared with predictions from the BEB model, excellent agreement is observed, provided that

TABLE VI. Experimental doubly differential ionization cross sections of the reference gas N₂. The DDCS are given in units of 10⁻¹⁶ cm²eV⁻¹sr⁻¹. Experimental uncertainties are estimated to be 15%.

$T = 60 \text{ eV}$				DDCS					
$E \text{ (eV)}$	25°	35°	45°	60°	75°	90°	105°	120°	135°
5	77	97	108	103	111	112	101	96	112
10	65	69	73	70	73	68	65	66	72
20	65	51	48	40	36	31	31	34	38
$T = 80 \text{ eV}$				DDCS					
$E \text{ (eV)}$	25°	35°	45°	60°	75°	90°	105°	120°	135°
5	112	98	126	112	110	106	101	99	100
10	74	66	86	75	71	67	63	61	58
20	43	36	46	36	32	28	25	25	25
30	50	34	38	25	19.6	15.8	15.3	16.4	18.2
$T = 100 \text{ eV}$				DDCS					
$E \text{ (eV)}$	25°	35°	45°	60°	75°	90°	105°	120°	135°
5	96	121	123	121	124	112	111	105	101
10	69	79	81	84	79	70	66	69	59
20	33	34	37	36	32	26	24	23	23
40	39	29	25	18.8	13.5	10.8	9.5	10.3	11.4
$T = 200 \text{ eV}$				DDCS					
$E \text{ (eV)}$	25°	35°	45°	60°	75°	90°	105°	120°	135°
5	92	132	132	116	105	103	91	84	72
10	61	73	75	76	69	67	57	54	46
20	31	30	32	35	30	26	24	19.2	16.7
40	10.5	10.7	12.9	12.9	9.8	7.7	6.7	5.4	4.9
60	7.6	8.1	8.8	7.9	4.8	3.7	2.9	2.7	2.7
80	10.4	8.9	7.9	5.5	3.2	2.3	1.91	1.70	1.87
$T = 400 \text{ eV}$				DDCS					
$E \text{ (eV)}$	25°	35°	45°	60°	75°	90°	105°	120°	135°
5	48	75	70	69	66	63	65	54	40
10	36	43	44	41	40	40	41	30	26
20	16.6	17.4	18.1	19.6	19.1	16.3	17.1	11.0	8.4
50	3.1	3.7	4.4	5.3	5.0	3.3	2.8	2.0	1.49
100	0.96	1.44	2.04	2.13	1.22	0.70	0.54	0.44	0.32
140	0.91	1.33	1.62	1.21	0.52	0.30	0.21	0.22	0.15
160	1.03	1.43	1.55	0.92	0.38	0.24	0.18	0.12	0.12
$T = 1 \text{ keV}$				DDCS					
$E \text{ (eV)}$	25°	35°	45°	60°	75°	90°	105°	120°	135°
5	34	33	29	22	29	45	39	31	22
10	19.4	16.6	16.2	12.7	17.9	28	22	17.8	13.1
20	7.2	6.5	6.7	5.5	8.2	12.3	9.4	6.8	4.7
50	0.94	1.10	1.31	1.32	2.1	2.9	1.73	1.16	0.76
100	0.23	0.31	0.41	0.52	0.72	0.70	0.36	0.24	0.17
200	0.07	0.10	0.15	0.23	0.19	0.12	0.06	0.04	0.04
300	0.06	0.07	0.13	0.12	0.06	0.04	0.02	0.01	0.02
400	0.07	0.09	0.14	0.06	0.02	0.02	0.01	0.01	0.01

rescaled orbital binding energies and mean kinetic energies are used, as proposed by Champion *et al.* [31].

Finally, total scattering cross sections of NH₃, estimated by summing the TECS and TICS, are in good agreement with the values recommended by Itikawa [2].

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DATA AVAILABILITY

The data that support the findings of this article are openly available [38].

APPENDIX A: EXPERIMENTAL CROSS SECTIONS OF AMMONIA

1. Experimental elastic scattering cross sections

In Table III, the present differential, total elastic scattering, and momentum transfer cross sections of NH₃ are provided.

2. Experimental doubly-differential electron-impact ionization cross sections

The following section provides tables with the doubly differential ionization cross sections (DDCS) of NH₃ (Table IV), and Table V presents the SDCS and TICS of NH₃.

APPENDIX B: EXPERIMENTAL CROSS SECTIONS OF THE NITROGEN REFERENCE

The reference gas used in the relative flow technique was nitrogen (N₂). The DCS and DDCS values were obtained in an independent experiment, which utilized a different methodology and helium as a reference gas [17]. Their consistency with other literature was thoroughly validated [39]. The DCS values are provided in Ref. [14]. The DDCSs are listed in Table VI.

- [1] S. Bang, R. Snoeckx, and M. S. Cha, Kinetic study for plasma assisted cracking of NH_3 : Approaches and challenges, *J. Phys. Chem. A* **127**, 1271 (2023).
- [2] Y. Itikawa, Cross sections for electron collisions with ammonia, *J. Phys. Chem. Ref. Data* **46**, 043103 (2017).
- [3] W. R. Harshbarger, A. Skerbele, and E. N. Lassettre, Generalized oscillator strength of the $\bar{A} \rightarrow \bar{X}$ transition of ammonia, *J. Chem. Phys.* **54**, 3784 (1971).
- [4] D. T. Alle, R. J. Gulley, S. J. Buckman, and M. J. Brunger, Elastic scattering of low-energy electrons from ammonia, *J. Phys. B: At. Mol. Opt. Phys.* **25**, 1533 (1992).
- [5] M. G. P. Homem, I. Iga, G. L. C. de Souza, A. I. Zanelato, L. E. Machado, J. R. Ferraz, A. S. dos Santos, L. M. Brescansin, R. R. Lucchese, and M. T. Lee, Electron collisions with ammonia and formamide in the low- and intermediate-energy ranges, *Phys. Rev. A* **90**, 062704 (2014).
- [6] R. El Mir, E. M. Casagrande, A. Naja, C. D. Cappello, S. Houamer, and F. E. Omar, Triple differential cross sections for the ionization of the valence states of NH_3 by electron impact, *J. Phys. B: At. Mol. Opt. Phys.* **48**, 175202 (2015).
- [7] R. El Mir, K. Kaja, A. Naja, E. M. Staicu Casagrande, S. Houamer, and C. Dal Cappello, New investigation of the electron-impact ionization of the intermediate valence state of ammonia, *J. Phys. B: At. Mol. Opt. Phys.* **54**, 015201 (2021).
- [8] R. Rejoub, B. G. Lindsay, and R. F. Stebbings, Electron-impact ionization of NH_3 and ND_3 , *J. Chem. Phys.* **115**, 5053 (2001).
- [9] Y. R. Choi, N. Sinha, M. Y. Song, D. C. Kim, Y. Kim, and Y. Park, Total cross section measurements of electron scattering from NH_3 in the intermediate-energy region, *Eur. Phys. J. D* **78**, 65 (2024).
- [10] F. Blanco and G. García, Screening corrections for calculation of electron scattering differential cross sections from polyatomic molecules, *Phys. Lett. A* **330**, 230 (2004).
- [11] F. Blanco, L. Ellis-Gibbins, and G. García, Screening corrections for the interference contributions to the electron and positron scattering cross sections from polyatomic molecules, *Chem. Phys. Lett.* **645**, 71 (2016).
- [12] R. Loch, B. Leyh, W. Denzer, G. Hagenow, and H. Baumgärtel, The photoionization of ammonia revisited. The vibrational autoionization of NH_3 and its three isotopomers in the 10-12 eV photon energy range, *Chem. Phys.* **155**, 407 (1991).
- [13] M. Dinger, W. Y. Baek, and H. Rabus, Comparative experimental and theoretical study on doubly differential electron-impact ionization cross sections of pyrimidine, *Phys. Rev. A* **109**, 062813 (2024).
- [14] M. Dinger, Y. Park, P. Hepperle, and W. Y. Baek, Combined experimental and theoretical study on the elastic electron scattering cross sections of ethanol, *Eur. Phys. J. D* **77**, 52 (2023).
- [15] S. K. Srivastava, A. Chutjian, and S. Trajmar, Absolute elastic differential electron scattering cross sections in the intermediate energy region. I. H_2 , *J. Chem. Phys.* **63**, 2659 (1975).
- [16] J. C. Nickel, P. W. Zetner, G. Shen, and S. Trajmar, Principles and procedures for determining absolute differential electron-molecule (atom) scattering cross sections, *J. Phys. E: Sci. Instrum.* **22**, 730 (1989).
- [17] W. Y. Baek, M. Bug, H. Rabus, E. Gargioni, and B. Grosswendt, Differential elastic and total electron scattering cross sections of tetrahydrofuran, *Phys. Rev. A* **86**, 032702 (2012).
- [18] D. W. Breck, *Zeolite Molecular Sieves: Structure, Chemistry, and Use* (Wiley, New York, 1973), p. 771.
- [19] N. Mehio, S. Dai, and D. E. Jiang, Quantum mechanical basis for kinetic diameters of small gaseous molecules, *J. Phys. Chem. A* **118**, 1150 (2014).
- [20] R. D. Dubois and M. E. Rudd, Differential cross sections for elastic scattering of electrons from argon, neon, nitrogen and carbon monoxide, *J. Phys. B: At. Mol. Phys.* **9**, 2657 (1976).
- [21] T. W. Shyn and G. R. Carignan, Angular distribution of electrons elastically scattered from gases: 1.5-400 eV on N_2 . II, *Phys. Rev. A* **22**, 923 (1980).
- [22] N. Sanna and F. A. Gianturco, Differential cross sections for electron/positron scattering from polyatomic molecules, *Comput. Phys. Commun.* **114**, 142 (1998).
- [23] N. Sanna and F. A. Gianturco, SCELlib: A parallel computational library of molecular properties in the single center approach, *Comput. Phys. Commun.* **128**, 139 (2000).
- [24] N. Sanna, I. Baccarelli, and G. Morelli, SCELlib3.0: The new revision of SCELlib, the parallel computational library of molecular properties in the single center approach, *Comput. Phys. Commun.* **180**, 2544 (2009).
- [25] A. I. Lozano, J. Rosado, F. Blanco, P. Limão-Vieira, and G. García, Integral electron scattering cross sections from N_2O for impact energies ranging from 1 to 1000 eV, *J. Phys. Chem. A* **128**, 699 (2024).
- [26] J. B. Furness and I. E. McCarthy, Semiphenomenological optical model for electron scattering on atoms, *J. Phys. B* **6**, 2280 (1973).
- [27] I. E. McCarthy and X. Zhang, Distorted-wave born approximation for electron-helium double differential ionisation cross sections, *J. Phys. B: At. Mol. Opt. Phys.* **22**, 2189 (1989).
- [28] S. J. Ward and J. H. Macek, Wave functions for continuum states of charged fragments, *Phys. Rev. A* **49**, 1049 (1994).
- [29] Y.-K. Kim and M. E. Rudd, Binary-Encounter-Dipole model for electron-impact ionization, *Phys. Rev. A* **50**, 3954 (1994).
- [30] Y. C. Wang, G. Visentin, L. G. Jiao, and S. Fritzsche, Acceleration correction to the binary-encounter bethe model for the electron-impact ionization of molecules, *Phys. Rev. A* **109**, 022804 (2024).
- [31] C. Champion, M. A. Quinto, and P. F. Weck, Electron- and proton-induced ionization of pyrimidine topical issue: COST action Nano-IBCT: Nano-scale processes behind ion-beam cancer therapy andrey solov'yov nigel mason, gustavo garcía and eugene surdutovich, *Eur. Phys. J. D* **69**, 127 (2015).
- [32] N. Sanna, I. Baccarelli, and G. Morelli, The VOLSCAT package for electron and positron scattering of molecular targets: A new high throughput approach to cross-section and resonances computation, *Comput. Phys. Commun.* **180**, 2550 (2009).
- [33] R. W. van Boeyen, N. Watanabe, J. W. Cooper, J. P. Doering, J. H. Moore, and M. A. Coplan, Two-step single-ionization mechanisms, *Phys. Rev. A* **73**, 032703 (2006).
- [34] M. Dürr, C. Dimopoulou, B. Najjari, A. Dorn, K. Bartschat, I. Bray, D. V. Fursa, Z. Chen, D. H. Madison, and J. Ullrich, Higher-order contributions observed in three-dimensional ($e, 2e$) cross-section measurements at 1-keV impact energy, *Phys. Rev. A* **77**, 032717 (2008).
- [35] Y. Wang, Y. J. Zhou, and L. G. Jiao, Second-order born effect in single ionization of argon by electron impact, *Chin. Phys. Lett.* **29**, 013401 (2012).

- [36] M. E. Rudd, Differential and total cross sections for ionization of helium and hydrogen by electrons, *Phys. Rev. A* **44**, 1644 (1991).
- [37] W. Y. Baek, M. U. Bug, H. Nettelbeck, and H. Rabus, Doubly differential cross sections for electron-impact ionization of propane in the energy range from 30 eV to 1 keV, *Eur. Phys. J. D* **73**, 61 (2019).
- [38] M. Dinger and W. Y. Baek, Electron-impact total, multiple-differential elastic and ionization cross sections of ammonia: A joint theoretical and experimental study [datasets], Zenodo (2025), doi: [10.5281/zenodo.15806024](https://doi.org/10.5281/zenodo.15806024).
- [39] M. Dinger, Y. Park, and W. Y. Baek, Elastic and inelastic electron scattering cross sections of trichlorofluoromethane, *Phys. Rev. A* **111**, 022809 (2025).