

Low-energy elastic scattering of positrons by N₂O

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We present a theoretical investigation on positron scattering by N₂O. Elastic differential and integral cross sections at both the static and static plus correlation-polarization levels of approximation are calculated and reported in the 0.1–100 eV. Calculations were performed using two theoretical methods, namely, the Schwinger multichannel method and the method of continued fractions. Also, two different schemes were used to treat correlation-polarization effects. The comparison between our calculated results and the existing experimental data is encouraging.

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I. INTRODUCTION

During the past two decades, investigations on physics and chemistry of matter-antimatter interactions have constituted subjects of increasing interest in the scientific community. Today, many sophisticated experimental studies including the production, storage, and manipulation of antimatter such as positrons [1], antineutrons [2], antiprotons [3], and antihydrogen atoms [4] are routinely performed in laboratories. Particularly, concerning the interaction of positrons with atoms and molecules, there is a set of interesting problems which are expected for further investigations such as the mechanisms of annihilation of thermal positrons [5,6] and the existence of positron-molecule bound states [7]. Special attention is focused on the dynamics of inelastic positron-molecule scattering channels, i.e., positronium formation, direct ionization, electronic excitation, and others. A more complete and comprehensive review on this matter is given by Surko *et al.* [8].

From the theoretical point of view, even elastic positron-molecule interactions are interesting. In contrast to electron-atom (molecule) interaction, exchange effects are absent for positrons, as the projectile and the target particles are distinguishable. Even though theoretical investigation of positron-molecule scattering remains a hard task, since the calculated cross sections would reflect a suitable balance between repulsive static and attractive correlation-polarization contributions of the interaction potential. Specifically, there are basically two ways to deal with the polarization effects. In the so-called *ab initio* methods, the many-body aspects of the interaction are taken explicitly into account. On the other hand, in *ad hoc* phenomenological methods, an one-particle parameter-free model correlation-polarization potential is used to represent the many-body aspects of the positron-molecule interaction. In this work both methodologies are

employed in order to extract useful information of the dynamics in elastic positron scattering.

In particular, the present study reports a theoretical investigation on elastic positron scattering by the N₂O molecule. More specifically, differential cross sections (DCS's) in the 0.1–100 eV energy range and integral cross sections (ICS's) in the 0.1–10 eV range for elastic positron-N₂O scattering are calculated and reported. Two different theoretical methods, namely, the Schwinger multichannel (SMC) method [9] and the method of continued fractions (MCF's) [10–12] are used to solve the Lippmann-Schwinger scattering equations. In SMC's, the polarization effects are treated using a full *ab initio* method whereas in MCF's such effects are accounted for by using a parameter-free model potential. Also, the influence of the formation of positronium is not considered in both calculations. As far as we know, the only existing theoretical study for positron scattering by this system was carried out by Baluja and Jain [13]. They reported total (elastic+inelastic) cross sections (TCS's) for incident energies above 10 eV. Therefore, collisions at lower energies were not accounted for. On the experimental side, relative DCS's for quasielastic (including rotational and vibrational excitations) positron-N₂O scattering in the 4–100 eV range were measured and reported by Przybyla *et al.* [14]. Also, TCS in the 1–500 eV incident energy range were reported by Kwan *et al.* [15]. These experimental results are compared to our calculated data. This comparison can provide an interesting insight of the elastic positron-N₂O interaction dynamic and can indicate the degree of reliability of the used methods.

This article is organized as follows. In Sec. II, we give an outline of the methods and procedures of computation. In Sec. III, we present our results and discussions and finally, in Sec. IV, we present our conclusions.

II. THEORY

In this section, we present the two theoretical methods used in our calculations. In both cases, the fixed-nuclei

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framework is used. The calculated DCS's are vibrationally and rotationally unresolved and therefore, can be compared directly with the experimental data of Przybyla *et al.* [14].

A. Schwinger multichannel method

We start with the Schwinger multichannel method. The application of SMC for positron-molecule scattering has already been discussed by Germano and Lima [9] and here, we just outline some expressions for the sake of completeness of this article. Atomic units are used throughout this work except when explicitly stated.

The backbone of the method is the computation of the variational expression for the scattering amplitude, which is given by

$$f_{\vec{k}_i \rightarrow \vec{k}_f}^{\text{SMC}} = -\frac{1}{2\pi} \sum_{mn} \langle S_{\vec{k}_f} | V | \chi_m \rangle (d^{-1})_{mn} \langle \chi_n | V | S_{\vec{k}_i} \rangle \quad (1)$$

with

$$d_{mn} = \langle \chi_m | PVP + Q\hat{H}Q - VG_p^{(+)}V | \chi_n \rangle, \quad (2)$$

where $S_{\vec{k}}$ is a solution of the unperturbed Hamiltonian (molecular Hamiltonian plus the kinetic energy operator of the incident positron), P and Q are projection operators, onto energetically open and closed states of the target, respectively, V is the interaction potential, \hat{H} is the total energy minus the scattering Hamiltonian, $G_p^{(+)}$ is the projected Green's function onto the P subspace, and $\{\chi_m\}$ are the $(N+1)$ -particle trial scattering functions.

In low-energy positron-molecule scattering, it is necessary to take into account polarization effects. SMC describes the target polarization through virtual single-particle excitations of the target, explicitly considered in the expansion of the scattering wave function

$$\Psi_{\vec{k}}^{(+)} = \sum_{\nu} \Phi_0(1, \dots, N) \varphi_{\nu}(p) + \sum_{\mu\nu} \Phi_{\mu}(1, \dots, N) \varphi_{\nu}(p), \quad (3)$$

where $\Phi_0(1, \dots, N)$ is the target ground state Hartree-Fock (HF) wave function, φ_{ν} are positron scattering orbitals and Φ_{μ} are singly excited target wave functions belonging to the closed channel Q subspace and are written as Slater determinants. The Q subspace (polarization space) is constructed considering all hole-particle excitations from occupied to the polarized orbitals [16], given as

$$\phi_{i,\alpha} = \sum_{j \neq i} \phi_j \frac{\langle \phi_j | \mu_{\alpha} | \phi_i \rangle}{E_j - E_i}, \quad (4)$$

where the sum runs over all virtual orbitals and E_j and E_i are orbital energies. μ_{α} is the α th component ($\alpha=x, y, z$) of the dipole moment operator. The use of polarized orbitals turns the size of the polarization space suitable for computational purposes.

Because SMC is a variational method, the quality of the calculated results would depend on the quality of the trial scattering basis set $\{\chi_m\}$. The lack of an upper-bound or a lower-bound limit for continuum scattering functions makes

particularly the choice of basis functions critical. Recently, Chaudhuri *et al.* [17] developed a methodology to treat numerical instabilities in the matrix elements of SMC along N_2 electronic excitation calculations. Later, Arretiche and Lima [18] applied this procedure, called the basis set Born approximation technique (BSBAT), to model electronic excitation of H_2 by positron impact obtaining convergence of calculated cross sections from different sets of scattering basis. Here, we apply the BSBAT to treat elastic positron- N_2O scattering.

B. Method of continued fractions

In the method of continued fractions, the positron-molecule collision problem is formulated in the body-fixed (BF) framework. The dynamics of the scattering can be appropriately represented by the BF Lippmann-Schwinger integral equation

$$\Psi = S + G_0 U \Psi, \quad (5)$$

where Ψ is the wave function of the positron, S is a set of solutions of the unperturbed Schrödinger equation, and U is the interaction potential. The Lippmann-Schwinger equation is solved by iteration using the method of continued fractions (MCFs) [10,11]. The application of MCFs consists of defining the n th-order weakened potential operator $U^{(n)}$ as

$$U^{(n)} = U^{(n-1)} - U^{(n-1)} | S^{(n-1)} \rangle \langle A^{(n-1)} |^{-1} \langle S^{(n-1)} | U^{(n-1)} \quad (6)$$

and the n th-order correction of $D^{(n)}$ matrix is defined through the relation

$$D^{(n)} = B^{(n)} + A^{(n)} [A^{(n)} - D^{(n+1)}]^{-1} A^{(n)}. \quad (7)$$

Here,

$$A^{(n)} = \langle S^{(n)} | U^{(n)} | S^{(n)} \rangle, \quad (8)$$

$$B^{(n)} = \langle S^{(n-1)} | U^{(n-1)} | S^{(n)} \rangle, \quad (9)$$

and

$$S^{(n)} = G_0^p U^{(n-1)} S^{(n-1)}. \quad (10)$$

The superindex p in the Green's function refers to the principal-value component.

The reactance matrix K is related to the D matrix through

$$K = -D. \quad (11)$$

The operator $U^{(n)}$ is expected to become weaker with increasing n . Generally, five steps are sufficient to reach the desirable convergence. When the convergence of the iterative procedure is achieved, the calculated reactance matrix K corresponds to the exact solution of the Lippmann-Schwinger equation. The transition matrix T is related to the K matrix through the expression

$$T = -\frac{2iK}{(1-iK)} \quad (12)$$

and the BF differential cross section (DCS) is given by

$$\frac{d\sigma}{d\Omega} = |f|^2, \quad (13)$$

where f is the BF elastic scattering amplitude related to the T matrix by the usual expression

$$f = -2\pi^2 T. \quad (14)$$

In order to compare the calculated cross sections with experimental data, a frame transformation on scattering amplitude is done in a conventional way [19]. The resulting laboratory-frame (LF) DCS, expanded in the j_t basis representation, after average of molecular orientations is

$$\frac{d\sigma}{d\Omega} = \sum_{j_t, m_t, m_t'} \frac{1}{2j_t + 1} |B_{m_t, m_t'}^{j_t}(k_0, k', \hat{r}')|^2, \quad (15)$$

where $\vec{j}_t = \vec{l}' - \vec{l}$ is the transferred angular momentum along the collision and m_t and m_t' are the projections of j_t along the laboratory and molecular axis, respectively. The $B_{m_t, m_t'}^{j_t}(\Omega')$ coefficient is given by

$$B_{m_t, m_t'}^{j_t}(\Omega') = \sum_{l' l m} (-1)^m a_{ll'm} (ll'0m_t | j_t m_t) \times (ll' m m' | j_t 0) Y_{lm}(\Omega'), \quad (16)$$

where the dynamical coefficients $a_{ll'm}$ can be written in terms of fixed-nuclei partial-wave components of the electronic portion of the transition matrix elements as

$$a_{ll'm}(k_0) = -\frac{1}{2} \pi [4\pi(2l'+1)]^{1/2} i^{l'(l'-l)} \langle k_0 l m | T | k_0 l' m \rangle. \quad (17)$$

Finally, in order to compare our data with the rotationally unresolved DCS for quasi-elastic e^+ -N₂O scattering, we calculate rotationally summed DCS's [20] as

$$\frac{d\sigma}{d\Omega} = \sum_{j=0} \frac{d\sigma}{d\Omega}(j \leftarrow j_0), \quad (18)$$

where j (j_0) are final (initial) rotational quantum numbers of the target. This procedure was employed for both methods (SMC and MCF).

The positron-molecule interaction potential in the body-frame fixed-nuclei approximation is formed by two components

$$U(\vec{r}) = U^{\text{st}}(\vec{r}) + U^{\text{CP}}(\vec{r}). \quad (19)$$

The static potential U^{st} , is the electrostatic term arising from Coulomb interactions between the projectile and the nuclei and electrons of target. The U^{CP} term is the correlation-polarization potential arising at short range from bound-free many-body effects and at long range from the induced polarization effects. In our calculation we use in the short range a parameter-free correlation potential U^{CP} proposed by Arponen and Pajane [21] and applied in positron-molecule scattering by Jain [22] and Jain and Gianturco [23]. The short-range part of the potential is related to the correlation and the long-range part is responsible for the polarization

$$U^{\text{CP}}(\vec{r}) = V_{\text{corr}}(\vec{r}) \quad \text{for } r \leq r_c \quad (20)$$

and

$$U^{\text{CP}}(\vec{r}) = V_p(\vec{r}) \quad \text{for } r \geq r_c, \quad (21)$$

where V_{corr} is the correlation potential, V_p is the polarization potential given by

$$V_p = -\frac{\alpha_0}{2r^4} - \frac{\alpha_2}{2r^4} P_2(\cos(\theta)) \quad (22)$$

and r_c is the radius where V_{corr} and V_p terms cross each other for the first time. This is the procedure to establish the cutoff and give the physically reasonable form at short and large r . Specifically, the cutoff parameter used in this calculation was 3.31 a.u. for $L=0$ and 2.49 a.u. for $L=2$. It is interesting to observe that with these cutoff parameters, we found that 92.7 and 71.6 % of the electronic charge were enclosed inside the correlation portion of the potential for $L=0$ and $L=2$, respectively. For $L=2$ there is a second point of intersection between the correlation potential and the polarization one. This point is located at 4.59 a.u. and evidently it incorporates practically all the electronic charge of the molecule. In fact, the choice of the matching point between the correlation and polarization components is rather arbitrary. In some test runs, we have learned that the influence of the $L=2$ component of the U^{CP} on the calculated cross sections is not relevant. Also, the use of different matching points does not affect significantly the calculated DCS's. Thus, the first crossing point between the correlation and polarization potentials was used in the present study. Moreover, partial-wave components with L larger than 2 are expected to be small and are neglected in this work.

C. Computational details

Following Lee *et al.* [20], the experimental equilibrium geometry of the ground state ($R_{N-N}=2.127a_0$ and $R_{N-O}=2.242a_0$) is used in the computation of the ground-state target wave function. The standard [9s5p/4s3p] basis sets of Dunning [24] augmented by one s ($\alpha=0.028$), one p ($\alpha=0.025$), and one d ($\alpha=0.8$) uncontracted function at the nitrogen centers and three s ($\alpha=0.025, 0.02$, and 0.005), one p ($\alpha=0.04$), and three d ($\alpha=1.7, 0.85$, and 0.34) functions at the oxygen center are employed in the HF self-consistent-field (SCF) calculations. This basis set gives a SCF energy of -183.726991 a.u. and a dipole moment of $0.6532D$ computed using the GAMESS code [25]. These values can be compared to the results -183.736716 a.u. and $0.6318D$ from the near-Hartree-Fock calculation of Winstead and McKoy [26]. This target wave function is used to generate interaction potential in both the SMC and MCF calculations. In order to generate the long-range polarization potential according to Eq. (20), we use the experimental values of the symmetric ($\alpha_0=20.22$ a.u.) and asymmetric ($\alpha_2=13.17$ a.u.) polarizabilities [27].

In the MCF calculations, the partial-wave expansion of both bound and continuum orbitals, as well as all the matrix elements required in the calculation, were retained at $l_{\text{max}}=47$ and $m_{\text{max}}=17$ for all incident positron energies. Some

truncation tests were carried out using the MCF. The tests showed that at large scattering angles the convergence of DCS was reached approximately for $l \approx 10$ and $m \approx 4$. For completeness, the single-center expansion was developed from the central nitrogen atom, which is located in the origin of the coordinate system. We used a radial grid of 900 points for integration, where the maximum value of the radial coordinate used R_{\max} was equal to 92 a.u. The use of this value guarantees the normalization of the outmost valence orbital to be better than 0.999 and also satisfy the scattering boundary condition.

In SMC, the positron scattering orbitals are taken from the set of Hartree-Fock orbitals, which are linear combinations of Gaussian functions of s , p , and d type. Because of that, the higher partial wave component that can be obtained from the scattering basis set is relatively small. Due to this fact, the DCS's converged, in general, for $l_{\max} \approx 5$. So, we think the choice for $l_{\max} = 9$ in SMC calculations is fairly satisfactory. Moreover, due to N_2O is a polar molecule, it is expected that the DCS near the forward direction is dominated by the dipole interactions. Such interactions are of very long range and must be corrected via a Born-closure procedure. Indeed, such procedure were performed in both the SMC and MCF calculations.

III. RESULTS AND DISCUSSION

In Fig. 1 we compare the DCS's calculated using the SMC and the MCF, respectively, at incident energies of 0.25, 0.5, 1, 1.5, 2, and 3 eV. The results calculated at both the static and the static plus correlation-polarization (SCP) levels are presented. In the absence of experimental data and other similar calculations, we expect that these data would be useful for further investigations in this energy region. For such low energies, it is expected that the correlation-polarization effects would play an important role in the dynamics of elastic $e^+ - N_2O$ collisions. In fact, it is seen from this figure that there is a significant difference between the calculated static and SCP DCS's using both the SMC and MCF methods, particularly for energies above 1 eV. Moreover, although there is a general good qualitative and quantitative agreement between the static results of the two calculations, some discrepancies are seen particularly in an angular range between 10° and 70° . This difference may be attributed to the lower partial wave component that can be reached in SMC calculations. The DCS's calculated at the SCP level of approximation by the two methods are also in general good agreement. In this case, the discrepancy seen between them, cannot be totally attributed to the different ways of accounting for the correlation-polarization effects.

In Fig. 2, we present the static and SCP DCS's calculated by both the SMC and the MCF at incident energies of 4, 6.75, and 10 eV. The relative quasielastic data of Przybyla *et al.* [14], normalized to our MCF SCP data at 60° is also shown for comparison. Again, the significant discrepancy between the corresponding SCP and static results evidences the importance of the correlation-polarization effects in this energy range. The good quantitative agreement between the SCP DCS's of the two methods shows the correlation polar-

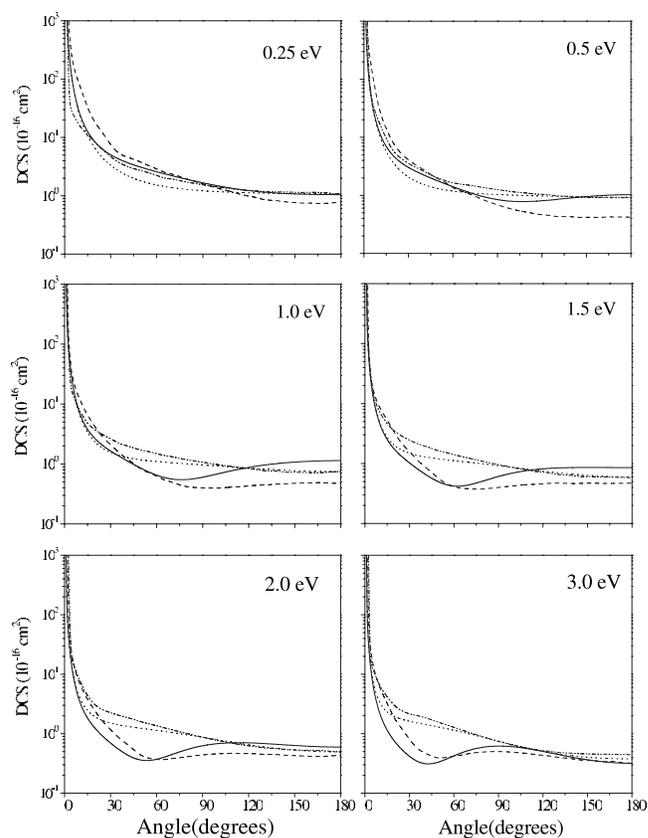


FIG. 1. Elastic differential cross sections for $e^+ + N_2O$ for 0.25, 0.5, 1, 1.5, 2, and 3 eV. Dashed-dotted line, static MCF results; dotted line, static SMC calculation; dashed line and full line, MCF and SMC calculations in static plus correlation-polarization approximations, respectively.

ization can be handled, for polar molecules, using both the *ab initio* treatment or model potentials. The comparison with the experimental data has shown that, in general, the angular dependence of the experimental DCS's at 4 and 10 eV is well described by both the SMC and MCF calculations at the SCP level of approximation. However, at 6.75 eV, the maximum seen in the experimental data at around 90° is shifted to small scattering angles in the calculated DCS. The proximity of this energy to the thresholds of the real positronium formation (6.02 eV) and electronic excitation of $^1\Delta$ (6.75 eV) [28], suggests that the observed discrepancy is due to the neglect of these effects in the present calculation, which is a single-channel one. We believe that further studies that include these specific inelastic channels can solve this question. For 4 and 6.75 eV, we observe that the experimental DCS's are larger than their theoretical counterparts at small scattering angles. This feature is not seen at higher incident energies. It is interesting to point out that a similar behavior was observed by de Carvalho *et al.* [29] for elastic $e^+ + N_2$ scattering and by Jain and Gianturco [30] for $e^+ + CH_4$ scattering. Apparently, more theoretical efforts, particularly for better description of the correlation-polarization effects, are needed in order to improved the calculated DCS near the forward direction. Also, more experimental attempts for positron-molecule scattering, particularly those performed by independent groups, are welcome.

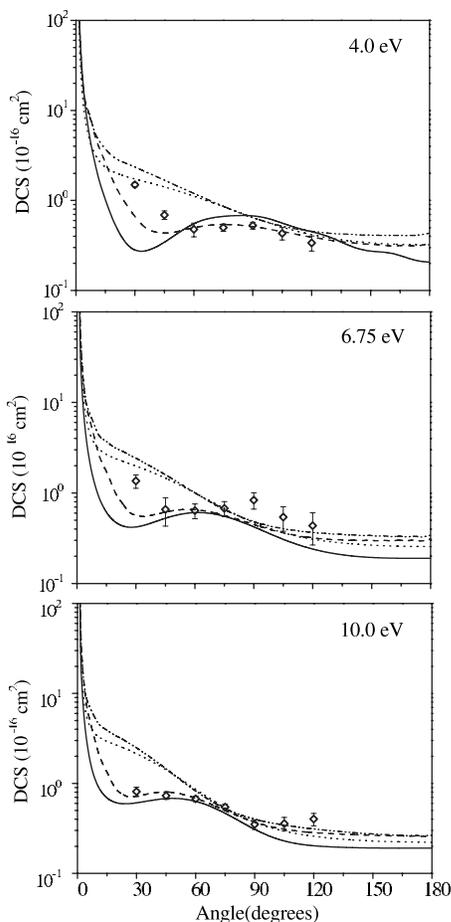


FIG. 2. Elastic differential cross sections for $e^+ + N_2O$ for 4.0, 6.75, and 10.0 eV. Theoretical legends are the same as in Fig. 1. Diamonds are the quasielastic measurements of Przybyla *et al.* [14].

In Fig. 3, we show the DCS's calculated at the static and SCP levels for 20, 50, and 100 eV incident energies. Only the results of the MCF theory are presented. For these energies, the comparison of our SCP data with the experimental data shows an excellent qualitative agreement, which is very encouraging. It is quite surprising to see that the role played by the correlation-polarization effects is still relevant for such energies. The influence of these effects in the calculated DCS's can be clearly seen at angles less than 30° . Particularly, a minimum feature is seen in the SCP data in this angular range. A previous study of electron- N_2O scattering [20] has shown that the correlation-polarization effects are significantly less important than for positrons, at incident energies above 20 eV. However, for positron scattering, the static and correlation-polarization components of the interaction potential present opposite signal. Therefore, probably the balance of the repulsive static and attractive correlation-polarization potentials has produced the observed minimum.

The reason for the omission of SMC results at these energies is due to the fact that our scattering basis sets are not "complete" for energies above 10 eV, as suggested by the BSBAT analysis. However, as the first application to a polar target, we are happy for its satisfactory description on the dynamics of the low-energy positron-molecule scattering.

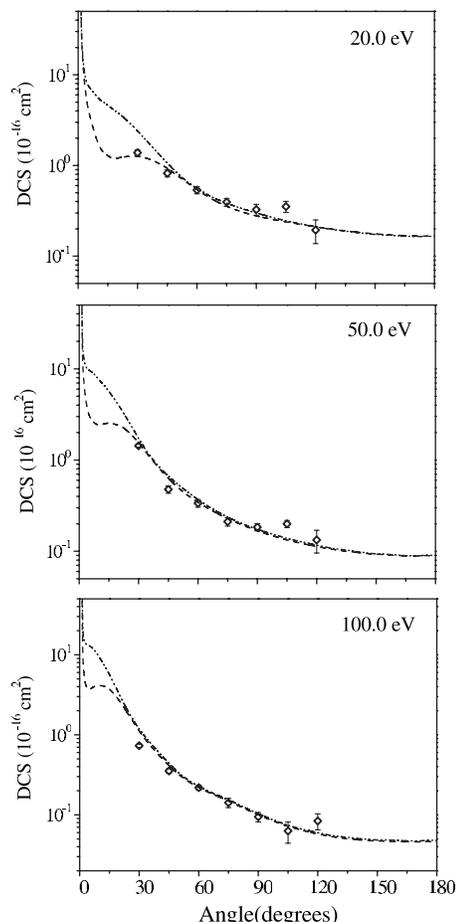


FIG. 3. Elastic differential cross sections for $e^+ + N_2O$ for 20.0, 50.0, and 100.0 eV. Dashed-dotted lines are static MCF calculations; dashed lines are static plus correlation-polarization MCF results; diamonds are the experimental data of Przybyla *et al.* [14].

Finally, the static and SCP ICSs in the 0.25–10 eV energy range, calculated using the SMC and MCF methods are presented in Fig. 4. The experimental TCS of Kwan *et al.* [15] is also shown for comparison. At such low incident energies, the elastic scattering channel dominates the interaction between the positron and target. Therefore, the comparison of our calculated ICS with the experimental TCS is meaningful. As expected from the analysis of the DCS's, the SCP ICS provided by the SMC and MCF methods agree quite well. Again, the small discrepancies seen between them can be attributed to the different manners to account for the correlation-polarization effects as well as different expansion parameters used in the calculations. The two sets of SCP results also agree quite well with the experimental TCS of Kwan *et al.* [15]. The similarity with our elastic results and the experimental TCS above 6.02 eV, which is the positronium formation threshold, suggests that this scattering channel has a small contribution to the total cross section. As expected, the static results calculated by the two methods deviate significantly from the SCP ICS and also from the experimental TCS, indicating again the importance of the role played by correlation-polarization effects in positron-molecule collision.

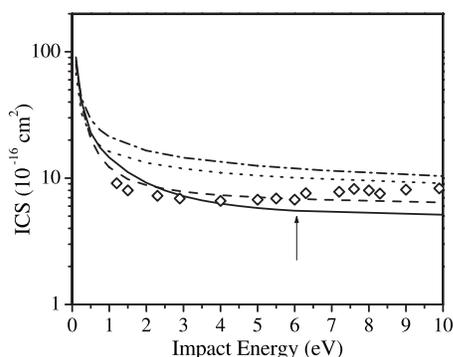


FIG. 4. Elastic integral cross sections for $e^+ + \text{N}_2\text{O}$. Dotted line and dot-dashed line are SMC and MCF calculations in the static approximation. Full line and dashed line are SMC and MCF results, respectively, in the static plus (correlation-)polarization approximation. Diamonds are the total cross section measurements of Kwan *et al.* [15]. The arrow indicates the positronium formation threshold.

IV. CONCLUSIONS

In this work, we report an application of the SMC and MCF methods to study $e^+ + \text{N}_2\text{O}$ scattering in the low- and intermediate-energy range. The calculations were performed in both the static and SCP levels of approximation. Two different calculation schemes, namely, the full *ab initio* method and a model potential method, were used to handle the correlation-polarization effects. As far as we know, this is the first time that different approaches to take into account po-

larization and correlation effects in low-energy positron elastic scattering are directly compared and mainly computed with the most similar initial conditions, this is, basis sets, molecular geometry, etc. We learned that both approaches can produce similar descriptions for the elastic cross sections for polar molecules. Also, the calculated cross sections using the SCP approximation agree fairly well with the experimental data available in the literature. On the other hand, the discrepancy between the theoretical and experimental DCS's at small scattering angles still remains as a problem to be better understood.

Another point is the important role played by the correlation-polarization effects at incident energies as high as 100 eV. This is probably due to the balance of the repulsive static potential and the attractive correlation-polarization potential.

Finally, it would be interesting to the positron-molecule research field if further DCS measurements, mainly in the low angle region, could be carried out by different experimental groups. The appearance of more experimental data would certainly stimulate theoreticians to look for improvements in the description of the positron-molecule scattering.

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