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Data for Modeling of Positron Collisions and Transport in Gases

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Abstract. We review the current status of positron cross sections for collisions with atoms and molecules from the viewpoint of their use in studies of positron transport processes in gases, liquids and human tissue. The data include cross sections for positron scattering in rare gases, molecular gases (eg., for N₂, H₂, CO₂, CF₄) and in particular for organic molecules and those relevant for applications in medicine (e.g. formic acid and water vapor). The cross sections were taken from an assessment of previously published positron-target cross sections. All of the cross sections are based on binary collision measurements and theoretical calculations, and they were not explicitly modified according to the standard swarm analysis. The main reason for this is systematic lack of experimental data for positron transport properties in gases. However, we believe that our compiled sets of cross sections are at level of sophistication, and of sufficient accuracy, to provide correct interpretation of future positron-based experiments. Using these cross sections as an input in our Monte Carlo simulations and Boltzmann equation treatment, we review some interesting points observed in the profiles of various transport coefficients for positrons in gases. Particular emphasis is placed upon the analysis of kinetic phenomena generated by the explicit influence of Ps formation.

Keywords: positron, cross sections, complete sets, swarm.

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INTRODUCTION

Positron physics is a rapidly growing area of research, interesting from both a fundamental [1] point of view, and because of applications that positrons have in many areas, ranging from material science [2] and medicine [3], to astrophysics [4]. In all of these applications, interactions with matter are required. Thus, in order to model any positron application, two types of data are necessary. The first type is collisional data, which gives information on positron scattering from individual atoms and molecules. In the last few decades, a revolutionary breakthrough in positron atomic physics was made by Surko *et al* [5, 6] who have developed the Penning–Malmerg buffer gas trap for positrons, which now can give high-intensity and high-resolution positron beams for measuring positron cross sections at low, and well-defined, energies [7-10]. The second type of data, which essentially relies on the knowledge of the cross sections for positron scattering, is data associated with the transport of

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charged particles through gaseous and soft condensed medium. This type of data gives the information about the group of charged particles traveling through the medium, such as their mean energy, drift and diffusion, range and thermalization. Unfortunately, there are limited experimental data on transport coefficients for positrons [11] and only a few groups in the world are directly involved in the modeling of positron transport. In order to model positron transport via Monte Carlo simulations, or by the Boltzmann equation analysis, complete sets of cross sections are a necessary input. The cross section set is said to be “complete” if it provides a good particle, momentum and energy balance in the so-called swarm limit.

When assessing the availability of electron and positron scattering data in the literature, it is obvious that there is much more information for electrons than for positrons. Before the development of Penning-Malmberg-Surko trap, it was very difficult to produce beams with sufficient numbers of positrons to make reliable measurements of cross sections for positron scattering, especially for lower energies and with high enough energy resolution. On the other hand, positron interactions with atoms and molecules are fundamentally different from interactions which involve electrons [1], and some of these differences make theoretical calculations of positron cross sections very difficult.

As the positron charge is opposite in sign to that of the electron it can always be distinguished from the electrons in the target (atom or molecule). As a consequence, there is no exchange interaction for positrons. The so-called static (Coulomb) interaction between the positron and atom is of the same magnitude as the static interaction of the electron, but with opposite sign (it is repulsive). The polarization potential, which attempts to model the polarization of the atomic charge cloud due to the incoming projectile, is attractive and of the same strength for both positrons and electrons. These two interactions tend to cancel each other for positrons, so the overall interaction with the atom is less attractive than for an electron. This is the reason why, at low energies where the polarization effect is dominant, the cross sections for positrons are (typically) significantly smaller than the cross sections for electrons [12].

At higher energies, where positronium (Ps) formation becomes possible, the complications for theory increase enormously. Ps formation is an extremely strong scattering channel and it must be included in any scattering calculation if meaningful results are to be expected. It poses a particular problem in that the final state in such a scattering calculation is multi-centred, and thus extremely difficult to treat exactly. Only a few calculations, using coupled channel approaches, have managed to do this with any level of accuracy.

At high enough energies, say around 1 keV, the polarization and exchange interactions become negligible and static potential dominates. This potential is the same magnitude for electrons and positrons and the cross sections for both particles become essentially the same, with the values given reasonably accurately by the first Born approximation [13]. The absence of the exchange interaction apparently makes theoretical treatment of positron scattering easier, but more careful analysis shows that there can be strong correlation effects between the target electrons and projectile positron which need to be taken into account. These correlations are the result of attractive electrostatic interaction between the positron and electron from the target

and can be treated as real or virtual states of positronium (Ps). Their role is much more important than the role that electron-electron correlations have in electron scattering.

At very low energies, the only open channels of interaction are annihilation and elastic scattering. With increasing positron energy, inelastic channels start to open: Ps formation, excitations of atomic levels and ionization. Ps can be formed in its ground states or any other energetically allowed excited state, while the target excitations are limited to those levels which do not require alteration of the spin, as exchange is not possible, and spin-orbit interaction for positrons has been shown to be negligible, even for heavy atomic systems. Direct annihilation is possible at all positron energies, but it has a cross section much smaller than cross sections for any other process. The necessary condition for Ps formation is that positron has energy greater than the difference between the threshold for ionization and the Ps binding energy (6.8 eV). If the target atom/molecule has ionization energy less than 6.8 eV, Ps can be formed even by positrons with zero energy.

In the context of swarm studies, Ps formation is a non-conservative process which leads to a loss of positrons from the swarm, and therefore it is, in some ways, analogous to electron attachment in electron transport. On the other hand, direct ionization does not increase the number of particles in the positron swarm and should be treated as a conservative inelastic process, although a separate analysis for electron swarms may be in order.

In this paper we review the available data on positron scattering cross sections and transport coefficients for positrons in neutral gases from the literature. We primarily focus on what we call "complete sets" of cross sections for positron scattering on Ar atoms and H₂, N₂ and CF₄ molecules, based on, to our knowledge, the best theoretical calculations and experimental measurements available in the literature. We are focused on the lower to intermediate energy range ($10^{-3} - 10^3$ eV). Using these sets of cross sections, we have calculated transport coefficients for positrons in these gases, and also in water vapour. We give a brief overview of their most important characteristics when both the electric and magnetic fields are present.

This paper does not claim to be a complete review of all the available data on positron scattering. Important information on positron scattering at high energies is missing. Also, the data on positron annihilation, which is a very important process for some applications, are not included in this review. Recently it has been suggested that cross section for Ps break-up [14-18] can have a magnitude comparable to cross sections for other important processes in the energy range considered in this paper. A more complete presentation will require a more extensive publication and should also have detailed critical evaluation of the data. We believe however that the moment is right to prepare such a review and also set up a database.

DATA FOR MODELING OF POSITRON INTERACTIONS WITH MATTER

The basic data required for modeling positron interactions with matter are complete cross section sets, which include cross sections for all relevant positron scattering processes. In general, these cross sections are the following: total cross section (σ_T),

momentum transfer cross section (σ_m), cross section for elastic scattering (σ_{el}), positronium (Ps) formation (σ_{Ps}), direct ionization (σ_i), cross sections for vibrational (σ_v), electronic (σ_{eexc}) and rotational (σ_r) excitations, and also differential cross sections (σ_{diff}). The cross section for direct annihilation is usually negligible compared to the cross section for Ps formation, and therefore, for most applications, it can be omitted from the complete set. For longer time development of low energy positron swarms it is necessary to include annihilation.

The need for complete sets of cross sections for electron scattering in plasma modeling has been recognized in the past and there are many recommended sets of cross sections for electron collisions in the literature [19-21]. Most of these sets were developed and tested using a swarm method. The swarm method falls into the category of 'inverse' problems in physics where the cross sections are adjusted until agreement is achieved between experimentally measured and theoretically calculated transport coefficients. The swarm methods of deriving cross sections, developed mainly by Phelps and collaborators [22, 23] and Crompton and collaborators [24], became accepted as competitive and complementary to other established techniques, such as crossed-beam or total attenuation experiments. This was particularly the case in the low energy range where these experimental techniques were faced with a wide range of systematic problems if absolute values of integral cross sections are required. In the case of positrons, however, there are no published and recommended sets of cross sections which have been developed and tested using a swarm method. The fact that, apart from a couple of attempts, there are no active positron swarm experiments is the main reason for this. Except some early attempts to measure positron mobility, [25-27] there are no experimental data on positron transport coefficients. Reviews of history, current status and future prospects of positron swarm experiments have been recently published by Charlton [11] and Petrović et al. [28].

Table 1 illustrates the current situation in the literature concerning collisional data for positrons. We list noble gases, some simple molecular gases, and more complicated molecules which play important roles in positron applications. The presence of a star (*) means that those data are available in the literature.

TABLE 1. Available data on positron collision cross sections.

Gas	σ_T	σ_m	σ_{el}	σ_{Ps}	σ_i	σ_v	σ_{eexc}	σ_r	σ_{diff}
Ar	*	*		*	*		*		*
He	*			*	*				*
Ne	*			*	*				*
Xe	*			*					*
Kr	*			*					*
H ₂	*			*	*	*	*		*
N ₂	*			*	*	*	*		*
O ₂	*			*	*			*	*
CO ₂	*		*	*	*	*			*
CF ₄	*				*	*			
SF ₆	*								
H ₂ O	*			*	*	*			
HCOOH	*			*					
CO	*			*	*	*	*		*
CH ₄	*				*				*
CH ₃ F	*								

CH ₂ F ₂	*	
CHF ₃	*	
NH ₃	*	
C ₂ H ₂	*	
SiH ₄	*	
N ₂ O	*	*

CURRENT DATABASE FOR POSITRON COLLISION CROSS-SECTIONS

Table 1. shows the availability of the scattering data for positron collisions with different gases. Among these gases, up to now, sufficiently complete sets of cross sections are available only for Ar, H₂, N₂, CF₄ and H₂O. In this section we present these cross section sets. They are compiled from, to the authors' knowledge, the best measured and calculated cross sections for positron interactions with atoms and molecules available in the literature, and where necessary, completed with cross sections for electronic collisions. All of these sets are compiled having in mind positron applications (<http://mail.ipb.ac.rs/~cep/ipb-cnp/ionsweb/database.htm>).

Rare gases

Most of the data on positron scattering from the rare gases in Table 1 are theoretical calculations and experimental measurements of total cross sections (Ar [29], He [30-36], Ne [29, 37-41], Kr [29]). Also, a considerable amount of mostly experimental work is dedicated to measurements of cross sections for Ps formation (Ar [8, 42-47], He [30, 35, 42-44, 48-52], Ne [8, 37, 42, 45, 46, 52-54], Xe [8, 42, 45, 47, 55-57], Kr [8, 42, 45, 47, 58]) and direct ionization (Ar [8], He [59], Ne [60]). Some measurements of the differential cross sections are available for all noble gases [61-64], but the only available data on electronic excitations to our knowledge are those for Ar [65] and He [66]. Thus, the only noble gas at the moment with a sufficiently complete set of cross sections for positron impact is argon.

Argon (Ar)

The complete set of cross sections recommended for modeling of positron interactions with Ar is given in Fig. 1. Elastic scattering is represented by the momentum transfer cross section [67]. The cross sections for the electronic excitation of two lowest lying 3p⁵4s J = 1 levels of argon are taken from [65]. These are the only two levels of 4s manifold that are accessible by positron excitation. We have also added in a cross section for positron impact excitation of higher singlet levels based on that for electron impact excitation of argon [68]. The Ps formation and ionization cross sections were taken from the work of Marler *et al.* [8].

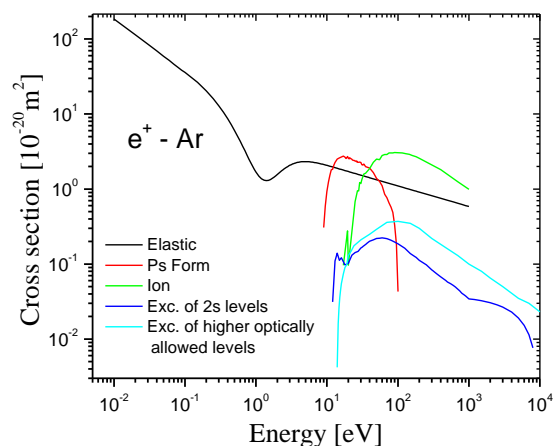


FIGURE 1. Cross sections for positron scattering in argon [68]. Sources of data are cited in the text.

Cross-sections for molecular gases

In the case of molecular gases, the great majority of work is again dedicated to measurements and calculations of total cross sections (H_2 [12, 70-72], N_2 [12, 70,73], O_2 [70, 71, 74-85], CO_2 [13, 42, 70, 71, 86-92], CF_4 [11, 70, 93], SF_6 [71, 81, 94], CO [70, 71], CH_4 [11, 70]), cross section for Ps formation (H_2 [88, 72, 95], N_2 [55, 82, 95], O_2 [82, 95], CO_2 [55, 91, 95-98], CO [82]) and direct ionization (H_2 [59, 88], N_2 [82, 99,100], O_2 [80, 82, 101], CO_2 [100, 102, 103], CF_4 [104], CO [82, 100, 103], CH_4 [100, 103]). For some of these gases the data on vibrational excitations (H_2 [105, 106], N_2 [107], CO_2 [105, 108, 109], CF_4 [82], CO [105]) and some measurements of electronic excitation cross sections (H_2 [67, 110], N_2 and CO [82]) are also available. When constructing the complete cross section set for some molecule, electronic excitations by positron impact can be replaced with appropriate cross sections for electron collisions, if the former are not available. The most important point here is that there is no exchange interaction for positrons, and therefore they cannot excite those states with a different total spin. As observed from Table 1, the data on differential cross sections for some molecules [92, 111, 112] can be found in the literature and also some theoretical work on rotational excitations [76].

In this section we discuss the complete sets of cross sections for N_2 , H_2 and CF_4 . It should be mentioned that the complete set of cross sections for CO_2 is just one step away, as the only missing data are those for electronic excitations. A similar situation exists for O_2 , where, apart from electronic excitations, the vibrational excitation data are also missing. While O_2 is important in positron physics of the upper atmosphere, CO_2 is interesting in atmospheric physics as the main factor in human induced greenhouse effect. The worst situation is with SF_6 , where the only available data are those for total cross sections [71, 81, 94]. SF_6 is often used as a cooling gas in positron traps, especially those employing the rotating wall technique [113]. Improvement and optimization of these traps requires the knowledge of cross sections for all individual positron scattering processes in SF_6 .

Nitrogen (N_2)

Fig. 2 shows the recommended set of cross sections for N_2 [114]. The total cross section was taken from the experimental measurements of Hoffman *et al.* [12] and we extended it below 1eV using the total elastic cross section calculated by de Carvalho *et al.* [73]. The cross sections for vibrational excitations were taken from theoretical work of Gianturco and Mukherjee [107], as there are no, sufficiently detailed, experimental data. Some errors were found in those calculations [105,106], and were corrected in [106]. According to the authors, corrections needed to be made only for H_2 , and therefore the data for vibrational excitations for N_2 could be taken from [107]. The cross sections for Ps formation and direct ionization were taken from Marler and Surko [82], while direct annihilation has been neglected. Finally, we have included the cross sections for the possible electronic excitations [82].

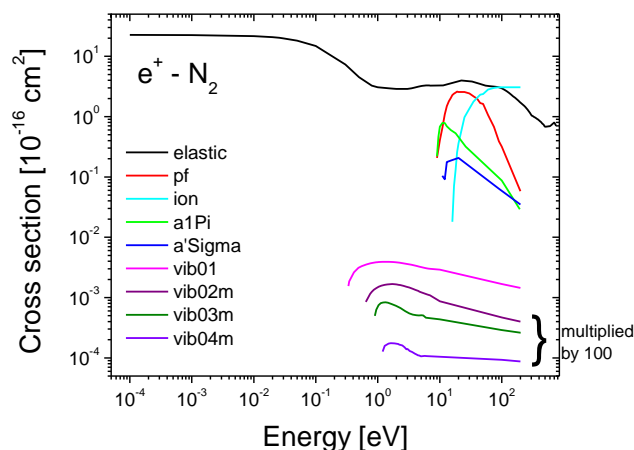


FIGURE 2. Cross sections for positron scattering in nitrogen. Sources of data are cited in the text [114].

Hydrogen (H_2)

In Fig. 3 the cross section set for positron interactions with molecular hydrogen is presented. The total cross section was taken from Hoffman *et al.* [12]. The cross sections for direct ionization and Ps formation were taken from experiments by Fromme *et al.* [88]. The cross section for electronic transition from the ground to lowest excited state, $X^1\Sigma_g^+ \rightarrow B^1\Sigma_u^+$ (X-B transition) has been measured in San Diego in the 11.19 – 30 eV energy range [65]. The cross sections for the next two excited states were taken from the theoretical considerations [110] as there are no reliable experimental results. The cross sections for vibrational excitations are also taken both from experiment (v1) [105] and the theory (v1,v3) of Gianturco and Mukherjee [106]. Cross sections for vibrational excitations for H_2 molecule calculated by Gianturco and Mukherjee, originally published in [107], had an error induced by the use of incorrect polarization parameters. The error was corrected in [106]. Elastic collisions are represented by the subtraction of the cross sections for all inelastic processes from the total cross section. All cross sections are extrapolated to 200 eV and direct

annihilation is neglected. The cross sections for rotational transitions are not included in this basic plot but are included in the set used in the transport data calculations. These cross sections (for non resonant excitation) can be easily calculated using the theory of Guerjov and Stein [115] for molecules without a dipole moment, and the Takayanagi theory [116] for those molecules possessing a permanent dipole moment.

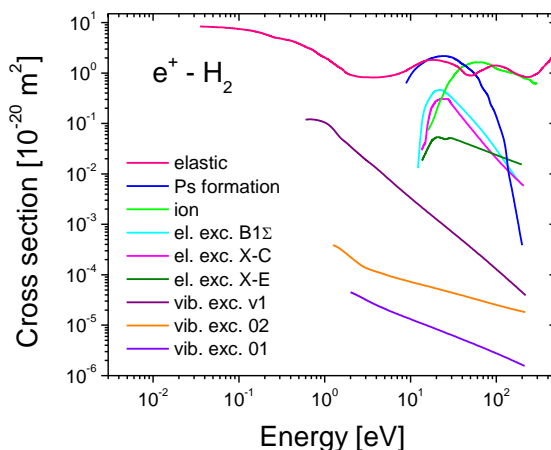


FIGURE 3. Cross sections for positron scattering in hydrogen [116]. Sources of data are cited in the text.

Tetrafluoromethane (CF₄)

The cross section set for positron interactions with CF₄ is given in Fig. 4. In creating this set we are mindful that CF₄ is often used as a cooling gas in Surko-type positron traps. This is not really a ‘complete set’, since some processes that may be relevant for the modeling of some other applications involving positron interactions with CF₄ are missing. However as this gas is used in the last (low energy) stage of thermalization in the Surko traps, the lack of electronic excitation cross sections, and an approximate estimate of the Ps formation cross section, are not critical factors. However, as there were suggestions [118] that CF₄ may be used as the sole trapping gas, and also for rotating wall applications, we have attempted to make the set as complete as it is presently possible.

This set includes cross sections for elastic collisions, Ps formation and inelastic processes (ionization and vibrational excitations). The total cross section is taken from the experiment of Makochekanwa *et al.* [13] and it covers the energy range 0.2 to 1000 eV. The elastic cross section is obtained by subtracting all inelastic cross sections from the total cross section. The total cross section is extrapolated to 0 eV using the theory of Nishimura and Gianturco [93]. The cross section for direct ionization is taken from the experiment of Moxom *et al.* [104]. To our knowledge, there is no data on the Ps formation cross section for CF₄ in the literature. Therefore we have used the cross section for Ps formation in Ar [8] shifted by the difference between the thresholds for this process in Ar and CF₄. The justification for this choice lies with the fact that cross sections for direct ionization are very similar in both shape and magnitude for Ar and CF₄. Thresholds for Ps formation in Ar and CF₄ are 8.955 eV [8] and 9.45 eV [13], respectively, so we added $\Delta = 0.495$ eV to the energy scale

of the cross section for Ar. This cross section set includes cross sections for three of four vibrational excitations [82]: v_1 ($E_{\text{exc}} = 0,113$ eV), v_3 ($E_{\text{exc}} = 0,159$ eV) and v_4 ($E_{\text{exc}} = 0,078$ eV). The cross section for vibrational excitation v_2 ($E_{\text{exc}} = 0,054$ eV) is omitted because neither experimental nor theoretical data exist for this transition. The energy range relevant for this process is still apparently out of reach for modern experiments [82]. The cross section for v_3 is measured in San Diego in the 0.1 – 2 eV energy range [82]. The cross section for v_1 excitation of CF_4 molecule by electron impact is also measured in the same energy range and using the same apparatus. This experiment revealed that vibrational cross sections for electrons and positrons in CF_4 are similar both in shape and magnitude, and this is confirmed by calculations based on the Born approximation. Having this in mind, we have extrapolated the cross section for the v_1 vibrational mode using results for electrons obtained by a swarm method [119]. Since positron data for vibrational modes v_1 and v_4 are missing, we have used the available data for electrons [119].

Electronic excitations of the CF_4 molecule induced by positron impact are also an important process to distinguish the percentage of trapped particles when CF_4 is one of primary cooling gases. These could not be included in the current set of cross sections for CF_4 due to the lack of data in the literature. One way to include electronic excitations into the cross section set is to take the effective cross sections for electronic dissociative excitations by electrons [19] and then to divide it by the factor of 4 [120]. Effectively we assume that cross sections for dissociation through repulsive states are similar and the difference in the magnitude is due to statistical weights.

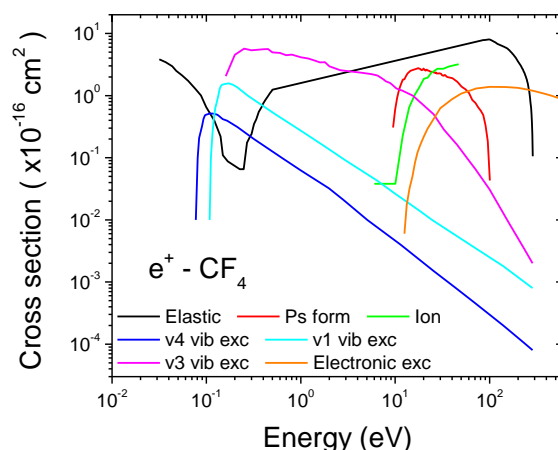


FIGURE 4. Cross sections for positron scattering in tetrafluoromethane. Sources of data are cited in the text.

Biologically relevant molecules

The most important potential application of positrons is in medical science, in particular to the diagnostic technique, Positron Emission Tomography (PET) [3], and the possible use of positrons in cancer therapy [121]. PET is a diagnostic technique widely used all over the world, with an assumption that it is non invasive and harmless

for humans. This assumption is not truly validated, and the details of positron interactions with human tissues on a molecular level are not yet well understood. This understanding can be achieved by modeling the interaction of positrons with living tissues and the first, and most important, step in this direction is to collect cross sections for all important positron interactions with relevant, biologically important molecules, in a wide energy range. The most important among these molecules is certainly water, since it is the main constituent of all living organisms. Indeed the human body is usually modeled as a “phantom” of appropriate geometry filled with liquid water. There exists a reasonable body of data on positron scattering from the water molecule, mostly in a lower energy range. The total cross section has been measured and calculated by a number of groups [10, 70, 122-130], and a similar situation exists for Ps formation cross section [10, 97, 131]. However, there is considerably less information on direct ionization, vibrational excitations, and angular differential cross sections. There are no measurements (or calculations) of cross sections for electronic excitations of the water molecule, but this problem can be avoided by using cross sections for appropriate electronic levels excited by electron impact. Another problem is how to deal theoretically with rotational excitations, since the water molecule has three axes of rotational symmetry. These cross sections cannot be measured because their energies are not in the range accessible to contemporary experiments. Based on data available in the literature, we have created a set of cross sections for positron scattering on the H₂O molecule. However, due to the importance of this molecule, the compilation and discussion of all the relevant cross sections for positron scattering on water are deferred to a future paper.

The next important molecule with some available data is formic acid. Formic acid (HCOOH) is the simplest organic acid, and is thought to play a major role in the formation of some larger biomolecules such as glycine and acetic acid. In addition, the derivative formate group (–COOH) is a key component of more complex biomolecules including some of the amino acids and DNA bases [132]. The only available data for formic acid, to our knowledge, are those for the total cross section [10, 132] and Ps formation [10]. Clearly, much more work needs to be done on measuring and calculating the cross sections for positrons in basic organic molecules before any serious simulations of living tissues can be done.

TRANSPORT PROPERTIES OF POSITRON SWARMS

In this section we briefly discuss the main features in the profiles of transport properties for positron swarms given as a function of the reduced electric and magnetic fields. More details can be found in our previous publications [68, 114, 117, 133-136]. A Monte Carlo simulation technique [68, 134], and multi-term theory for solving Boltzmann's equation [137], were used to calculate various transport properties under conditions critical for applications. Cross sections for positron scattering presented in this paper enter into the calculations as input data. Two essentially different techniques were necessary in order to validate and verify the results, because experimental measurements of the corresponding transport data do not exist. The obtained agreement is very good. The behavior of positron swarms was

studied under the influence of a dc electric field and in the crossed configuration of electric and magnetic fields, $\mathbf{E} \times \mathbf{B}$, in Ar [69, 133, 134], H₂ [117, 134], N₂ [114, 134] and H₂O [135]. The values of electric field were chosen in such a way to cover the energy range where all the important processes, given in the cross section sets, are active. On the other hand, the range of magnetic field strengths was chosen carefully for all individual gases to consider transport processes in three distinct regions of swarm behavior: (1) the collision dominated regime where the collision frequency dominates the cyclotron frequency; (2) the intermediate region where the collision and cyclotron frequencies are almost the same; and (3) the magnetic-field-guided region where the cyclotron frequency is much higher than the collision frequency [138-141]. Regardless of the field configuration and considered regimes, special attention was paid to the explicit influence of Ps formation on various transport coefficients.

Profiles of the mean energy were given as a function of E/n_0 (where E stands for electric field and n_0 for gas number density) for all considered gases. Among many interesting features, these profiles reflect the energy dependence of the cross sections. It was shown that drift velocity profiles show a remarkable sensitivity to non-conservative Ps formation; the difference between the flux and bulk components exceeds, in some cases, more than two orders of magnitude. A very pronounced negative differential conductivity (NDC) is observed in the profiles of the bulk drift velocity component for positrons in Ar, H₂ and H₂O [69, 114, 117, 133-135]. This phenomenon originates from the non-conservative nature of Ps formation and it is essentially different from the NDC effect observed in electron transport [142-144] in many aspects. The analysis of the diffusion coefficients shows an even higher sensitivity of the longitudinal diffusion with respect to the explicit influence of Ps formation. On the other hand, the transverse diffusion coefficient was only slightly affected by Ps formation. The only exception from these general trends so far is the drift velocity of a positron swarm in N₂ [113, 134], where the $a^1\Pi$ electronic excitation [82] has a threshold just before the opening of the Ps formation channel. Therefore the majority of positrons with energies close to these thresholds excite this electronic level, which has a reasonably large cross section, lose some of their energy and stay in the swarm. As a consequence, the difference between flux and bulk drift velocities of positrons in N₂ is much smaller than in other gases. The same applies for flux and bulk components of the longitudinal diffusion coefficient. The relative position of the thresholds for $a^1\Pi$ electronic excitation and Ps formation, and also the comparable magnitudes of these cross sections, make N₂ a good buffer gas for positron gas traps.

In a $\mathbf{E} \times \mathbf{B}$ field configuration the number of transport coefficients is increased. The drift velocity has two independent components along the \mathbf{E} and $\mathbf{E} \times \mathbf{B}$ directions, while the diffusion tensor has three different diagonal components, in the \mathbf{E} , $\mathbf{E} \times \mathbf{B}$ and \mathbf{B} direction. Independently of the type of gases, the effect of magnetic cooling was observed. However, perhaps one of the most striking phenomena in a $\mathbf{E} \times \mathbf{B}$ field configuration is an apparent disappearance of the NDC effect from the bulk profiles of the drift speed, while it is still present in the longitudinal component. This is even more interesting if the profiles of the drift velocity components and the profiles of the gradient energy vector are considered as a function of electric and magnetic field strengths. For positrons in Ar, H₂ and H₂O [117, 133, 135], due to the combined effects of magnetic field and Ps formation, the bulk component of the longitudinal

drift velocity component is more affected than the bulk component of the transverse drift velocity component. This, in turn, enhances the contribution of the transverse bulk component in the bulk drift speed and unexpectedly removes NDC from the profiles of the drift speed. The behavior of the diagonal elements of the diffusion tensor is also interesting. As an illustrative example, we would like to emphasize here that different diagonal elements exhibit different sensitivity with respect to the explicit influence of Ps formation and magnetic field. The most sensitive to Ps formation is the longitudinal diffusion coefficient, while the diffusion coefficient along the magnetic field direction shows very little sensitivity with respect to the effects of the magnetic field.

CONCLUSION

In this paper we have discussed the availability of cross section data for positron scattering from atoms and molecules in the literature. One of the key elements in optimizing positron-based technologies is the knowledge of complete sets of cross sections for positron scattering in gases. Complete sets of positron cross sections are available at the moment for the following gases: Ar, N₂, H₂ and H₂O. In this paper we have discussed the details of the cross sections for elastic and inelastic scattering of positrons in Ar, N₂ and H₂, and particular attention was paid to cross sections for Ps formation in these gases. The cross sections for positron scattering in water vapour are not discussed due to lack of space in this short review, and this is deferred to a future publication.

The cross sections presented in this paper were used as an input in Monte Carlo simulations and Boltzmann equation analysis of positron transport to calculate various transport properties under the influence of electric and magnetic fields. The most interesting points observed in the profiles of the various transport coefficients with electric and magnetic field strengths are identified and briefly discussed. While the modern theory of non-conservative transport did not exist when initial attempts were made to run positron swarm experiments it has now reached the level of sophistication and phenomenology required to explain the observed effects, and extract useful data. Thus it would be interesting to see whether it will be possible to revise this activity mainly as the benchmark for cross section sets.

The work on creating the data bases on positron cross sections has just begun. At this point it is extremely important that atomic and molecular physicists, who measure and calculate cross sections for positrons, work closely together with those who need their data in order to model the increasing number of positron applications. As an illustrative example, the most urgent data needed are the cross sections for electronic and vibrational excitations for O₂ and CO₂, having in mind the applications of positrons in atmospheric physics. In addition, one ought to mention an urgent need for the cross sections of positron scattering in SF₆ - often used in positron traps as a cooling gas. It is also crucial to understand that these models require complete sets of cross sections which provide good particle, momentum and energy balance in the system of consideration. The 'completeness' of the cross section sets can be tested using the swarm method. This suggests that it is necessary to build and run positron

swarm experiments. Only the cross section sets that can reproduce experimentally measured transport coefficients can be viewed as confident input parameters to model complex positron applications in realistic geometries. Apart from this, the recent calculations of positron transport parameters have revealed many new interesting kinetic phenomena, which crave experimental confirmation.

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