This manuscript was accepted by J. Phys. Chem. Ref. Data. Click here to see the version of record.

Recommended Positron Scattering Cross Sections for Atomic Systems

Kuru Ratnavelu[1], Michael J. Brunger[2] and Stephen J. Buckman[3]

[1]Institute of Mathematical Sciences, University of Malaya, Kuala Lumpur, Malaysia
and
Institute for Mathematical Research, Universiti Putra Malaysia, 43400 Serdang, Malaysia

[2]College of Science and Engineering, Flinders University, Adelaide, South Australia

[3]Research School of Physics and Engineering, The Australian National University, Canberra, Australia

ABSTRACT: We present a critical analysis of available experimental and theoretical cross section data for positron scattering from atomic systems. From this analysis we present (where data is available) recommended cross sections for total scattering, positronium formation, inelastic scattering and direct ionization processes. A complete bibliography of available measurement and theory is also presented.

TABLE OF CONTENTS

1. INTRODUCTION

1.1 Background to the Review

Positron and electron (lepton) scattering from gas-phase atoms and molecules are both mature experimental research fields which provide data for fundamental tests of quantum-based scattering calculations, as well as much-needed data for a host of applications in technology, medicine and the environment (e.g. [1]). Indeed, for electron interactions the major motivation in recent years has been the need for accurate and extensive cross section data, for all available processes, in order to model the role of electron-driven chemistry in a range of gaseous electronics environments such as lights and lasers, plasma processing and deposition, medical plasmas and environmental or atmospheric applications. Another key area of growth and need for electron-molecule scattering data has been in radiation damage and dosimetry following the discovery that low energy electrons can be a major cause of molecular damage in the body [2].

The field of positron interactions with atoms and molecules in the gas phase presents considerably greater challenges, given the difficulty in producing high flux, high energy resolution beams of positrons. Indeed, conventional techniques using radioactive sources and metallic moderators usually result in positron beam intensities which are many orders of magnitude lower than those obtainable with conventional electron beam technology, and an energy resolution which is, at best, about 150 meV [3]. Notwithstanding these difficulties, many important studies of positron-atom and positron-molecule interactions have been undertaken over the past 40 years, yielding absolute cross sections for a range of scattering processes [see e.g. 4].

The past several decades have witnessed somewhat of a renaissance in the field of positron scattering with higher flux, higher energy resolution beams becoming available as a result of higher activity radioactive sources and the, realised, potential of even higher flux beams from reactor-based sources. Perhaps the biggest advance for normal laboratory-based studies has come as a result of the development of rare-gas-moderated, trap-based positron beams, and associated measurement techniques [5,6], which have achieved higher fluxes and higher energy resolution than previous techniques. The advent of this technology has enabled improvements in the accuracy of absolute measurements and, with energy resolution of less than 50 meV readily achievable, it has opened up possibilities for study of vibrational and electronic excitation [e.g. 7,8], amongst other processes.

The other driver for this increased activity in positron scattering, and the associated technology developments, has been the applications of positron interactions in medical science and nanomaterials analysis. The key to these applications lies mainly in the formation and subsequent annihilation of positronium – a short-lived electron-positron pair, formed with high probability at energies below 100 eV, when a positron interacts with, and ionises, an atom or molecule. Positrons are now widely used in most major hospitals in the diagnostic technique Positron Emission Tomography (PET), yet little is known of "positron dosimetry" or the interactions that a high energy positron undergoes in the body when thermalising, through scattering, from several hundred keV to the low energies required for positronium formation and subsequent annihilation. The role of positron and positronium transport is not well understood in these environments, and so much of the recent work in this area has focused on interactions with biologically relevant molecules [9,10].

1.2 Previous Review Articles

There have been a number of previous "review" articles involving cross sections for positron interactions with atoms and molecules and, to the best of our knowledge, none of these have provided tabulated cross section values or recommended cross sections, with the notable exception of the recent review article by Chiari and Zecca [11], which we discuss below. However they do provide an excellent overall background to the field, including details of experimental and theoretical techniques – which we only consider briefly in this article in order to provide overall context.

The first substantive review of positron interactions was by Griffith and Heyland in 1978 [12], where current experimental and theoretical techniques and results were discussed, but no tabulated values were presented. Kauppila and Stein also reviewed the current status of positron scattering in both 1982 [13] and 1990 [14] with a particular interest in comparing electron and positron scattering cross sections for similarities and differences. A similar approach was adopted by Kimura and colleagues in their review [4]. Charlton and Humberston [15] provided a comprehensive discussion of all aspects of positron and positronium physics in their book "Positron Physics" in 2001 but did not provide tabulated values of cross sections. Surko *et al.* reviewed experimental and theoretical aspects of positron scattering and annihilation in their 2005 review article [16] but they also did not provide tabulated values or recommended cross sections.

In 2008 Laricchia and colleagues [17] reviewed the situation for positron impact ionization of atoms and molecules and discussed the level of agreement between experiments and experiment and theory but did not tabulate results. Recently, Danielson and colleagues reviewed trap-based techniques as applied to a range of antimatter experiments [18].

Finally, and of direct relevance to the present work, Chiari and Zecca reviewed positron scattering by atomic targets [11]. They provided recommended, tabulated cross sections for total scattering in the rare gases He, Ne, Ar, Kr and Xe, and a recommended positronium formation and total ionization cross section for He. While they discuss the relative merits of measurements of positronium formation and ionization for Ne – Xe, they do not recommend cross sections for these processes and gases, due largely to the significant spread in the published data. They also discuss measurements for other atomic systems – H, the alkalis and alkaline earth atoms. We also note our sister publication to this work which concerned tabulations of recommended cross sections for positron-molecule scattering [19].

1.3 Scope of this Review

In this article we are endeavouring to provide a comprehensive collection and assessment of the available experimental data (cross sections) for low- and intermediate-energy (0.1 eV – 1 keV) positron interactions with atoms. As mentioned above, in a previous article we provided a similar collection of data for positron-molecule scattering. This is not always an easy task when considering the available published data, as the positron community has not been noted for publishing tabulated values of measured cross sections, and this is particularly the case amongst the earlier measurements. Where more than one set of data is available for a particular target/scattering process, we have also attempted to provide what we consider to be the best "recommended" cross section. This, of course, is a risky task which is fraught with issues, not the least of which may be perceptions of bias – we have tried our best to minimise any such perceptions, and hopefully give a clear explanation of any rationale that has been

used in selecting recommended values. And, while we do not provide tabulated values of theoretical calculations of positron scattering cross sections, we do discuss and compare experiment and theory where it is possible for a given target, and we often use theory in guiding our determination of a "recommended" cross section.

The recommended cross sections are presented as smooth curves in the figures, with error estimates provided also as smooth curves, and the corresponding absolute values are given in tables in each section. It is hoped that in this fashion the data can be useful for any modeling applications that requires positron cross sections or as a ready reference for new theory or experiment, with the latter hopefully further refining the "recommended" sets.

This article is organised in the following manner. In sections 2 and 3 we give a brief overview of the experimental and theoretical approaches, respectively. Section 4 provides data and evaluation for positron scattering cross from atomic systems and these are presented in tabular form, and with an accompanying figure. Finally we provide an extensive list of references at the end of the paper.

This manuscript was accepted by J. Phys. Chem. Ref. Data. Click here to see the version of record.

2. EXPERIMENTAL APPROACHES

It is not our intention in this article to extensively review the nature of the cross section measurements or the experimental apparatus and techniques that have been used over the past (almost) 50 years to investigate positron interactions with atoms and molecules. That has been done, and done well, in a number of previous review articles [4, 11-14] and other major articles and books in the field [15-17]. However a brief summary of the various techniques that have been used to measure the processes discussed in this article - total, positronium, ionization and inelastic scattering cross sections – is relevant, as most techniques have both advantages and drawbacks, and these can be useful to keep in mind when assessing data for a "recommended" cross section. We will not discuss the rich collection of work on positron sources, moderators and detection schemes, but again refer the reader to previous work [e.g. 15,16].

2.1 Total Scattering

By far the most prevalent quantity measured for positron scattering is the Total Cross Section (TCS), sometimes also called the Grand Total Cross Section, and it is a measure of the total probability of scattering, irrespective of process, energy loss or scattering angle. It is an important quantity as generally it can be measured with high accuracy, and often provides a 'first point-of-contact' between experiment and theory.

The vast majority of total scattering measurements use the so-called attenuation technique, where the attenuation (loss) of positrons from a beam as it traverses a scattering cell containing the gas of interest is measured. The Beer-Lambert law is then commonly used to extract the total cross section from the measured attenuation fraction, the length of the scattering cell used (L), and the number density of the gas under study (N). The total cross section, usually labeled Q_T is given by

$$Q_T = \ln\left(\frac{I_0}{I_t}\right)\frac{1}{NL}$$

where I_0 and I_t are the transmitted positron fluxes, with no gas in the cell, and with gas, respectively.

Recent applications of this technique have produced accurate cross section measurements with absolute uncertainties as low as 3%. However there are a number of drawbacks to the attenuation technique that need to be considered when assessing data, with perhaps the most important of these relating to the effects of forward scattering on the measurements. These effects arise because the experiments are gas-dynamic, with the target gas (and positrons) flowing into and out of the scattering cell through entrance and exit apertures. The finite size of the exit aperture, in particular, means that some forward scattered positrons will always be present in the measured quantity I_T, and as a consequence this can result in a measured cross section which is lower than the "real" value. We will not discuss this particular issue further as it has been the subject of much recent analysis and discussion [e.g. 20], but it is important to note that it is thought to be one of the major reasons for some of the significant discrepancies that exist amongst literature values for total scattering cross sections. We do note that this effect can be a particular problem for target atoms and molecules which have

large dipole polarizabilities and/or dipole moments for molecules, as this generally translates into strong forward scattering.

2.2 Positronium Formation

Positronium (Ps) formation is perhaps the major inelastic process in low to intermediate energy (0-100 eV) positron scattering from most targets. It results in the loss of a positron from the incident beam and the production of a positive ion and either two or three gamma rays depending on the total spin of the positronium complex before it annihilates. Given the range of reaction products, there are also a range of techniques that have been used to measure, or estimate, the Ps formation cross section. In summary these are

- Measuring the loss of positrons from the incident positron beam
- Coincident detection of the two or three gamma rays that result from the annihilation of para- and ortho-positronium respectively
- Techniques which measure both the total ionization cross section (that is direct ionization plus Ps formation) and the direct ionization cross section in order to unravel the Ps formation cross section.

These techniques have had varying degrees of success and accuracy, although the best contemporary measurements typically have absolute uncertainties of around 5%.

2.3 Inelastic Scattering

There are relatively few measurements of inelastic scattering cross sections following positron excitation, with the majority either the result of time-of-flight (ToF) experiments or, more recently, experiments utilising trap-based beams in high magnetic fields.

In the ToF experiments [e.g. 21,22], a pulsed positron beam is used and inelastically scattered positrons are separated temporally from those scattered elastically. Not surprisingly these experiments were particularly challenging, with low fluxes and difficult absolute normalization.

On the other hand, trap-based experiments have provided a direct means to measure absolute, integral inelastic cross sections for many processes, including vibrational and electronic excitation. By manipulating the magnetic field strengths between the scattering and energy-analysing regions in these experiments, inelastic processes can be separated from elastic scattering, allowing the determination of cross sections using the Beer-Lambert law [23].

2.4 Direct Ionization

Given that there are two mechanisms which can lead to ionization by positron impact, positronium formation and direct ionization, techniques for measuring the direct ionization component must effectively separate these two mechanisms.

Early measurements of direct ionization also used ToF techniques to temporally separate positrons that had lost energy in an ionization event (e.g. [24]). Subsequent experiments have used more sophisticated coincidence techniques, where scattered positrons and positive ions are detected in coincidence (e.g. [25]). Buffer gas trap experiments have also served to improve the accuracy of direct ionization measurements [23]. A comprehensive review of

ionization techniques and cross sections was given recently by [17] and also discussed by [11].

3. OVERVIEW OF THEORETICAL METHODS

3.1 Introduction

Theoretical approaches in positron scattering by atoms and molecules have seen much progress since the early calculations by Massey and co-workers [e.g. 26,27]. However, even in the simplest case of the positron-hydrogen atom scattering system, the early theoretical methods were unable to treat the positronium formation (Ps) channel except by variational methods ([28] and references therein) which were limited for energies below the Ps formation and ionization threshold.

The early calculations such as the close-coupling approaches used the same computational codes as for the electron-atom case with a simple change of sign for the positron case and the polarization potential as well as ignoring exchange. However, these calculations neglected the rearrangement channels for Ps formation. In the positron case, the positron-electron correlations in the form of virtual and real Ps formation requires a much more complicated description to obtain accurate results for various scattering parameters.

In the last thirty years, there has been tremendous advancement of theoretical studies for positron-atom scattering, particularly in the inclusion of the Ps effects correctly. Coupled with the emergence of cheap and powerful computing resources, the tractability of various positron scattering from the simplest H atom to larger inert atoms has seen much success!

For much of the earlier and present state of theoretical methods on positron-atom scattering, there is a wealth of information from a number of previous reviews [11,13,15,16,29,30]. In particular, the recent review by Kadyrov and Bray [30] gives a detailed overview of the state-of-the-art in theoretical development. In the case of positron-molecule scattering, the following reviews provide useful and current information [11,15,16,31-34].

This present theoretical overview will briefly focus on these advances and the state-of-the-art theoretical methods of the last twenty years.

3.2 Close-coupling Methods

Close-coupling or the coupled-channels (CC) method and its variants such as the highly effective convergent close-coupling (CCC) and CC with pseudostates methods are considered the most successful theoretical techniques to study positron scattering from atoms, especially hydrogenic-type atoms at low to intermediate energies.

As noted above, the early idea of extending the basic single-centre close-coupling formalism to the positron case which only considered changing the sign of the incident particle, was valid for energies where Ps formation is insignificant. Here, the CC method expands the total wavefunction $\Psi(r_1, r_2)$ into an infinite number of orthogonal eigenstates of the target atom $\psi_\alpha(r_2)$. That is

$$\Psi(r_1, r_2) = \sum_\alpha F_\alpha(r_1)\psi_\alpha(r_2), \qquad (1)$$

where r_1 and r_2 are the coordinates of the scattered positron and atomic electron respectively. The eigenstates have unknown scattering coefficients $F_\alpha(r_1)$ which can, in principle, be obtained by solving a set of coupled integro-differential equations.

However at low and intermediate energies, the Ps formation channel plays a significant role in the scattering dynamics. Since the late 1980s, the CC methods have been able to treat the Ps formation channels for positron-atom scattering [35-39].

In the two-centre close-coupling formalism, the total wavefunction of the positron-atom collision system can be expanded in terms of the orthogonal eigenstates of the target atom ψ_α and Ps state φ_β with the corresponding unknown scattering coefficients F_α and G_β:

$$\Psi(r_1, r_2) = \sum_\alpha F_\alpha(r_1)\psi_\alpha(r_2) + \sum_\beta G_\beta(R)\varphi_\beta(s), \qquad (2)$$

where R is the centre of mass of the outgoing Ps atom and s is the relative coordinate, while α and β represent the channels in the atom and Ps respectively. These calculations were denoted by the CC(m,n) notation where m is the number of atomic states in the expansion and n is the number of Ps states used.

The challenge for the CC methods is in incorporating the maximum number of physical channels that can be included but to avoid weak convergence as the continuum channels are neglected. Eventually, these neglected effects were addressed by the development of CCC and to some extent earlier by the use of pseudostates and optical potential approaches.

3.2.1 Close-Coupling or Coupled-channel Calculations

Traditionally, close-coupling methods and its variants have been extensively used to study the electron (or positron) scattering on atoms [40-43]. Among these older calculations, Ward *et. al* [41-43] used a 2-state, 4-state and 5-state CC (CC2, CC4, CC5) on positron scattering from Li, Na and K. McEachran *et. al* [44] had also reported a 5-state CC calculation for positron scattering from Rb. We must also highlight a multi-pseudostate CC work by Walters [45] who used the 1s, 2s, 2p physical and 6 pseudostates of Fon *et. al* [46] to report positron scattering by H atom at intermediate energies.

In parallel, we witnessed the first set of two-centre CC calculations by Hewitt *et. al* [47,48] on Ps formation in positron-hydrogen scattering. They were the first to demonstrate a realistic CC calculation with the inclusion of the Ps channels in the eigenfunction of the total wavefunction. In this context, some early pioneering two-centre CC calculation works of Basu *et. al* [49,50], Wakid and Labahn [51] and Abdel Raouf *et .al* [52] must be mentioned.

Subsequently, Mitroy [37,53] implemented the CC in momentum space (denoted by CC(m,n), m-number of physical and pseudostates for the atomic channels and n-number of physical and pseudostates to represent the Ps channel) to obtain converged cross sections for various physical parameters in the positron-H system. Later, Mitroy and co-workers had also extended the CC(m,n) to study positron-sodium scattering [54,55]. Unlike the restrictive number of channels used in the earlier works [47-52], the CC(m,n) method allows for larger basis-state (using a L^2 formalism) calculations such as the 31-state CC(28,3) work of Mitroy

[53] for positron-H atom scattering. The corresponding work for the R-matrix approach will be discussed later.

3.2.2 Convergent Close-Coupling Method (CCC)

The CCC is considered one of the most effective methods in dealing with the issues of convergence and the handling of the neglected continuum states in the CC methods. It was developed by Bray and Stelbovics [56] for handling the formidable electron-hydrogen atom system. Essentially, the CCC uses square integrable (L^2) states which allow for a large number of physical and continuum channels to be used with ease in the eigenfunction expansion of the wavefunction. These eigenstates were obtained by diagonalising the target Hamiltonian in a large Laguerre or also Sturmian basis.

The first single-centre CCC calculation on positron-hydrogen atom was reported by Bray and Stelbovics in [57,58]. Other single-centre CCC calculations have been comprehensively detailed in Kadyrov and Bray [30] and will not be mentioned here.

Eventually, Kadyrov and Bray [59, 39] reported a two-center CCC implementation in positron-hydrogen atom scattering. Using the method of Mitroy [37], they extended the CCC formalism of Bray and Stelbovics [56] to calculate the total, elastic, break-up, ionization and Ps formation cross sections in the S-wave model.

Other two-centre CCC works include positron scattering by helium [60], lithium [61], sodium [62], magnesium [63] and H_2 [64]. Several physical parameters such as TCS, and the differential cross section (DCS) for positron scattering by neon, argon, xenon and krypton were calculated using the single centre CCC [65-67].

3.2.3 Coupled-channel optical methods (CCO)

During the period spanning the 1960-1990s, optical potential methods had been useful to treat the neglected discrete or continuum channels in a practically tractable calculation in electron-atom physics. Its utility was seen by a number of researchers (McCarthy, Saha and Stelbovics [68] and references therein).

The CCO's optical potential is derived from the Schrodinger equation using the Feshbach formalism [69]. Here, the reaction space is separated into 2 spaces, P space and Q space. The P space consists of atomic states whereas the Q space consists of continuum and remaining discrete states. The CCOM of McCarthy and Stelbovics [70] used an ab-initio complex-polarization potentials for the continnum effects and the remaining significant discrete channels were treated by second-order polarization potentials. Based on its success in e-H systems (McCarthy and Stelbovics) [70], a simple extension was implemented by Bransden *et. al* [71] for the positron-H system. Nevertheless, to be an effective method to treat the Ps formation, the optical potential must also include the neglected Ps formation. McCarthy, Ratnavelu and Zhou and McCarthy and Zhou [72,73] developed an equivalent optical potential to allow for these Ps formation channels.

In the late 1990s, Ratnavelu and Rajagopal [74] demonstrated an optical potential method (CCO(m,n)), within the CC two-centre formalism of Mitroy [37], that allowed for the

continuum optical potentials in the positron-atom channels. Using a small basis calculation (CC(3,3) and CCO(3,3)), they reported ionization cross sections, Ps formation cross sections and total cross sections that were in good qualitative and reasonable quantitative agreement with the 31-state CC calculations of Mitroy [75] and the 33-state R-matrix calculations of Kernoghan *et. al* [76]. Various implementations of the CCO(m,n) for positron-hydrogenic atoms were also reported [77-82].

In parallel, Zhou, McCarthy and Ratnavelu [83] developed the CCOM with a complex equivalent local potential, which treated the neglected atomic states and allowed for the Ps formation channels. In a series of calculations, Zhou and co-workers reported the CCOM for positron-alkali as well as positron-helium and positron-magnesium scattering [84-86].

3.3 *R*-matrix

One of the techniques used in theoretical studies of atomic, molecular and nuclear processes is the *R*-matrix theory [87,88]. This method was originally used to study the electron-atom collision processes by the Queen's University of Belfast group. For an overview of the R-matrix and its applications, the reader is referred to [89].

In the R-matrix approach, the configuration space of the physical system under study is divided into several parts and the system is solved separately in each of these domains. The wavefunction of the scattering system is represented by two parts - the internal and the external wavefunctions. The matching of these functions at the internal edge would give us the physical solutions' that is needed to generate the K-matrix [90].

The first realistic *R*-matrix calculation that allowed for the Ps channels was reported by Higgins *et al.* [90] in a study of positron-hydrogen scattering. They used the intermediate energy R-matrix method (IERM) with L^2 basis terms. Details of the development and implementation of the continuum Ps channels in the expansion of the total wavefunction were reported in Higgins and Burke [36, 91]. These allowed for overcoming convergence issues as well as to calculate the Ps(1s) cross sections. Further work by Walters and co-workers had extended this method to the positron-hydrogen, positron-alkali atom and positron-helium scattering systems [38,76,92-95].

A hybrid R-matrix [96] method for electron-impact ionization of atoms and ions was also extended to positron impact ionization of heavy noble gases [97]. This hybrid method used a first-order distorted wave (DW) to represent the incident positron and the initial bound state and the physics of the residual ion and ejected electron was treated by an R-matrix approach.

3.4 Relativistic Optical Potential Calculations

Even with the advent of highly sophisticated CCC and CC calculations, the role played by various perturbative methods in positron scattering by atoms in recent years particularly in positron scattering of inert gases is very significant [98-100, 65-67].

Chen *et.al* [98] proposed a relativistic optical potential method (ROP) to study elastic electron and positron scattering from noble gases. They derived a non-local ab-initio absorption potential within the Dirac relativistic formalism. Their imaginary part of the complex optical potential allowed for the fluxes of the neglected inelastic channels as well as the continuum

channels. The earlier model used by Bartschat *et. al* [101,102] had studied it in the non-relativistic formalism and did not allow for the continuum channels.

Following Chen *et. al* [98], the optical potential part of the coupled equations can be written as

$$U_{opt}(x)\begin{pmatrix} F_0(r) \\ G_0(r) \end{pmatrix} = \left[U^R_{opt}(r) - iU^I_{opt}(r)\right]\begin{pmatrix} F_0(r) \\ G_0(r) \end{pmatrix}$$

where $F_0(x)$ $G_0(x)$ are the elastic scattering functions and $U^R_{opt}(r)$ is the real part and $U^I_{opt}(r)$ is the imaginary part of the potential. The real part of the optical potential is approximated by the local polarization potential based on the polarized orbital potential of McEachran and Stauffer [103]. The polarization multipoles (ν=0 to 7) and dynamic distortion terms (up to 6 terms) as in McEachran and Stauffer [104] were used. The imaginary optical potential contribution was handled using a Hulthen-Kohn prescription that treats the complex part as a perturbation to reduce the tedious iterative process that is otherwise needed.

Jones *et al.* [65] used the ROP in the study of positron scattering from Ne and Ar to calculate the grand total cross section (GTCS) for Ne below the Ps threshold and above the threshold. Their work was comparable with other theories reported. In the Ar case, the ROP's GTCS showed poorer agreement with the experimental measurements. This was also reflected by other theories. The Ps formation cross sections also showed poor agreement.

Machacek *et al.* [66] had reported the ROP calculations for low energy calculations of positron scattering by xenon. We should note that the ROP as well as the CCC did not allow for the two-center treatment for handling the positron-atom scattering and were not able to describe the physics of the scattering at the Ps formation threshold such as the Wigner cusps. The ROP work in the positron-Kr process also did not show any improved results [67].

In 2013, McEachran and Stauffer [100] reported an implementation of the ROP that allowed for the Ps formation in the absorption channel following the procedures of Reid and Wahedra [105-106]. The Ps formation cross sections for Ne, Ar, Kr and Xe were calculated. These cross sections gave better results than other previous theoretical methods.

3.5 Other Optical-Model Potential, Born and Distorted-Wave Methods

There have been other optical potential approaches that were used to study positron scattering from atoms, such as the work of Gianturco and Melissa [107]. They reported Ps formation cross sections for positron scattering from Li, Na and K. Their method used a global modelling technique for the polarization potential, a generalized damping function for the short-range effects, and a dispersion relation for the absorption potential within a Feshbach formalism.

Reid and Wahedra [105] employed the parameter-free model potentials to study positron-K and positron-Rb scattering. Their method incorporated the absorption potential based on a

quasi-free model of Reid and Wahedra [106] and showed reasonable agreement with the experimental TCS data.

Another optical potential method is due to Garcia and co-workers [e.g. 108], where they implemented a version of the quasi-free absorption potential [109] for positron scattering by using the Reid and Wahedra prescription [106,110]. Further, they proposed an *ab-initio* absorption potential. In this approach, they derived the potential of the excited bound states and continuum in a Dirac-Fock formalism [98 and references therein]. In their calculation for Ar [108], a total of 17 bound states and 36 continuum channels were incorporated together with the inner-shell ionization. Perhaps the most important of the this groups' work is that within the independent atom method (IAM) and their screening-corrected additivity-rule (SCAR) plus interference (I) terms approach [e.g. 111,112], where their positron-atom optical model can be applied to molecular systems. Indeed, as shown in our companion paper to this review [19], the IAM-SCAR+I approach to positron-molecule scattering has been relatively successful in giving a semi-quantitative description of these scattering systems.

Recently, Bhatia [113] had proposed a hybrid theory to calculate accurate phase shifts, annihilation cross-sections and Ps formation cross sections for positron-H scattering at energies below the ionization threshold. His calculated phase shifts provide lower bounds to exact phase shifts.

There have been other theoretical methods that should be mentioned, for completeness. Gien [114-118] had used the modified Glauber (MG) approximation in the model potential approach to study positron scattering from several alkali atoms. His approach allowed for the inclusion of core-exchange effects which simplified the calculation of electron or positron scattering from hydrogenic atoms.

Other DW methods have been used extensively for positron-atom scattering in the late 1980s [119 and references therein]. Pangantiwar and Srivastava [120] had applied the DW method to positron-rubidium scattering. We also note the First Born (FBA) and distorted wave Born approximation (DWBA) calculations of Nahar and Wahedra [121,122]. They reported DCS and ICS for Ps formation from Li and Na at energies between 100-300 eV using both the FBA and DWBA methods. Their work on elastic scattering of positrons from Ar atoms at 3-300 eV needed model potentials for the lower partial-waves and Born approximations. Their reported DCS at 100-300 eV showed limited agreement with normalised experimental data [122].

Le *et al.* [123] implemented the hyperspherical close-coupling (HSCC) method for the positron-Li and positron-Na scattering systems. They extended the HSCC work on ion-atom scattering [124] and considered the hyperspherical radius of the collision adiabatically following the Born-Oppenheimer prescription. They also incorporated the positronic bound state effects using model potentials as in Ryzkhih *et. al* [125].

Campeanu *et al.* [126] used the DW method to calculate the ionization cross section for positron-H and positron-noble gas atom scattering. They used the Coulomb plus plane waves with full energy range (CPE) method, and the distorted CPE(DCPE) version to calculate the scattering T-matrix. In particular, the DCPE4 model of Campeanu *et al.* [127] gave results that looked quite promising. A newer model DCPE5 was later proposed in 2002 [128].

3.6 Many-body Theory Calculations

Green *et al.* [129] used the many-body theoretical (MBT) framework, based on the Dyson equation, to study positron scattering and annihilation by inert gases below the Ps formation threshold. Details of the MBT formalism can be found in Green *et al.* and its associated references. In particular, the MBT allowed for the electron-electron and electron-positron correlations to be calculated via perturbative techniques (via the Feynman diagrams). Additionally, the virtual Ps formation was incorporated using the prescription of Gribakin and King [130].

3.7 Variational Calculations

Variational techniques were employed by Hulthen [131] and Kohn [132] to evaluate scattering phase shifts and were extensively used in bound-state problems. In the 1960s', Schwartz [133] and Armstead [134] had reported elaborate variational calculations on elastic positron-hydrogen scattering. Due to issues such as the non-boundness of the phase shifts at non-zero energies, this led to further work by others. Bhatia *et al.* [135,136] had applied the lower bound formalism of Gailitis [137] to obtain rigorous lower bound calculations of s- and p-wave phase shifts for the positron-H case. These are considered to be exact. Stein and Sternlicht[138] used the Kohn and Hulthen method to study positron-H rearrangement collisions by extending it beyond the Ps formation threshold. Humberston and co-workers [139-142] and Houston and Drachman [143] also reported accurate phase-shifts for s-, p- and d-waves, as well as the corresponding cross sections. Another work by Humberston *et al.* [144] reported the 'round cusp' in the s-wave scattering cross section at threshold, in accord with Wigner's threshold theory.

There were some highly sophisticated variational calculations by Humberston and van Reeth that studied positron scattering by helium and hydrogen [145,146] in the low-energy region. In the positron-helium case, the variational *K*-matrix was calculated to energies below the first excitation threshold. An accurate form of the helium wavefunction, together with trial functions, were utilized with three variants of the Kohn variational method being reported - Kohn, Inverse Kohn and Complex Kohn. These trial functions would allow for the short-range effects. This work is considered as an important benchmark below the Ore gap for positron-He interactions.

In the positron-H case, accurate cross sections were also reported for the elastic scattering and Ps formation cross sections. These calculations, that used elaborate trial functions, showed interesting threshold structures due to the coupling between the Ps channels and the elastic channel. The s-wave Wigner cusp was also observed in their work.

This manuscript was accepted by J. Phys. Chem. Ref. Data. Click here to see the version of record.

4. RECOMMENDED CROSS SECTIONS FOR ATOMIC SPECIES

4.1 Atomic Hydrogen - H

Atomic hydrogen (H) is a notoriously difficult target to prepare for accurate quantitative scattering measurements in the laboratory. To our knowledge there have only been a few experimental determinations of absolute cross sections for positron scattering by atomic hydrogen, and these include measurements of the total scattering cross section [147-149], the positronium formation cross section [148,150-152] and the direct ionization cross section (which does not include Ps formation) [151-154].

4.1.1 Total Scattering

The total scattering cross section measurements for H have been done exclusively by the Wayne State group with their most recent efforts [148,149], representing their final, updated cross section. These measurements were carried out using a gas cell and a molecular hydrogen (Slevin) discharge as the source of the atomic target, and the Beer-Lambert law was used in an otherwise conventional attenuation experiment approach. The absolute normalisation of the cross section at a given energy was achieved by using the total cross section for H_2 at the same energy, together with a range of other measured experimental parameters. While there are no other experimental values with which to compare, when compared (see e.g. [16]) with several state-of-the-art theoretical approaches [56,75,95,142,155] the agreement between experiment and theory is excellent at energies above about 8 eV. The Wayne state group discuss possible forward scattering effects in their measured cross sections, and provide estimates of the extent that these may effect the measured cross sections. We are of the view that their low energy data, below 10 eV, considerably underestimates the true cross section due to these effects. As a consequence, our recommended cross section values at these lower energies, drawn largely from theory, are significantly higher than the measured experimental values. The recommended cross sections are given in Table 4.1.1 and shown in Figure 4.1.1. We estimate that the uncertainty in these cross sections values is around ±20%, particularly at the lower energies.

4.1.2 Positronium Formation

A variety of experimental techniques have been used to determine the positronium formation cross section for atomic hydrogen. A number of experiments in the Brookhaven-Bielefeld collaboration were carried out during the 1990's [150-152] with final values for the Ps formation cross section being provided by [152]. They used a crossed beam configuration and ion detection scheme to derive both Ps formation and impact ionization cross sections with absolute normalisation being provided via concurrent electron ionization measurements which were normalised to earlier literature values [156].

A different range of techniques was employed by the Wayne State group [148] to obtain the Ps formation cross sections. They measured both annihilation gamma rays, and the loss of transmitted positrons in their scattering cell, in order to estimate upper and lower limits on the Ps formation cross section, respectively. The absolute normalisation relies implicitly on measurements of total scattering for H and total and Ps formation for H_2 (see the original paper for details).

The Ps formation cross sections from these two groups provide a challenge when assessing a recommended cross section. The earlier results [150,151] favour a cross section with a peak amplitude around or above 3 $Å^2$, and the results of [151] are largely in good agreement with the later work from Wayne State [148]. However, the more recent result of the Bielefeld-Brookhaven collaboration [152], which they claim is an improved measurement to that of [151], indicates a cross section with a lower peak magnitude – around 2 $Å^2$. We can seek some guidance in this case from theory where there are now many reasonably reliable calculations of Ps formation. The majority of these predict a cross section with a peak maximum of around 3$Å^2$, so we are inclined to favour the data of [148] and [151], with the important caveat of a conservative uncertainty estimate of ±30% on the recommended cross sections. These values are tabulated in Table 4.1.2 and shown in Figure 4.1.2.

4.1.3 Direct Ionization

For positron impact ionization, the results of [152] were intended to supercede those of [151,153] from the same group/collaboration. These later results from the Bielefeld/Brookhaven collaboration are in good agreement with the results of the UCL group [154], which were undertaken primarily to validate the earlier measurements of [153], which were considerably larger than most contemporary theoretical calculations of the ionization process. Given the good agreement between the results of [152] and [154], and between these results and contemporary theory [58,75,76], our recommended cross section is largely based around these data. The cross sections are tabulated in Table 4.1.3 and shown in Figure 4.1.3, with an estimated uncertainty of ±25%.

Table 4.1.1: The total cross section (in units of 10^{-16} cm^2) for positron scattering from atomic hydrogen. The estimated uncertainty is ±20% (see also Fig. 4.1.1).

E_0 (eV)	Recommended TCS (x10^{-16} cm^2)
1.0	1.97
2.0	1.11
3.0	0.93
4.0	0.90
5.0	0.91
6.0	0.97
7.0	1.26
8.0	2.08
9.0	2.82
10.0	3.36
11.0	3.77
13.0	4.34
16.0	5.02
21.0	4.83
31.0	4.04
51.0	3.00
76.0	2.32
101.0	1.90
151.0	1.45
201.0	1.23
301.0	1.02

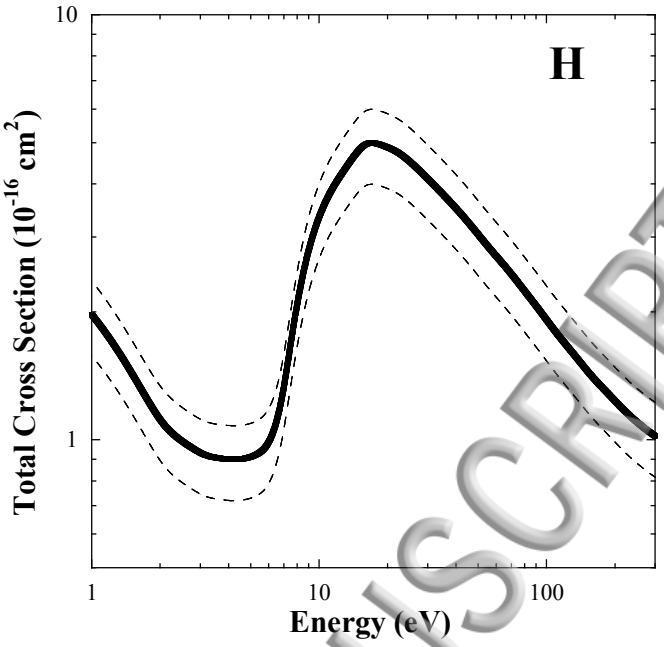

Figure 4.1.1. The recommended total scattering cross section for H (solid line), while the dashed lines represent the estimated uncertainty limits of ±20% (see also Table 4.1.1)

Table 4.1.2: Positronium formation cross section (in units of 10^{-16} cm^2) for atomic hydrogen. The estimated uncertainty is ±30% (see also Fig. 4.1.2).

E_0 (eV)	Recommended Positronium Formation Cross Section ($x10^{-16}$ cm^2)
7.0	0.568
8.0	1.08
9.0	1.68
10	1.94
11	2.36
12	2.77
13	2.93
16	2.93
18	2.70
20	2.45
25	1.94
30	1.48
40	0.91
50	0.56
75	0.14
100	0.035

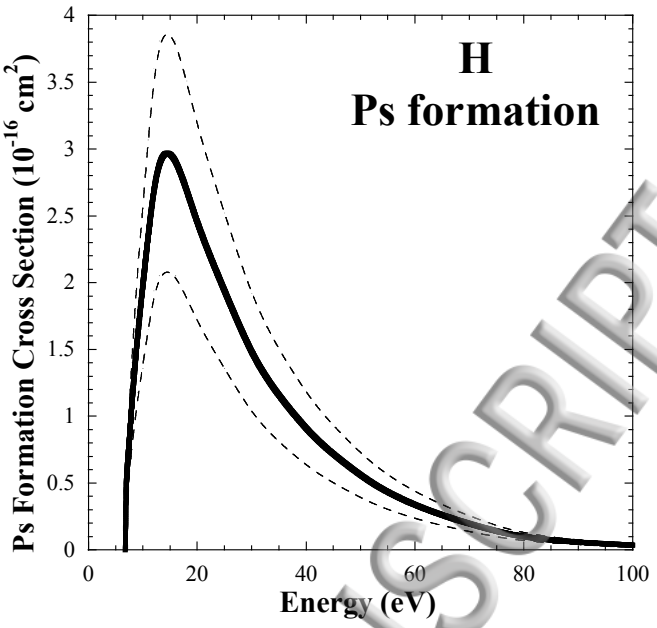

Figure 4.1.2. The recommended positronium formation cross section for H - solid line. The dashed lines represent the estimated uncertainty limits of ±30% (see also Table 4.1.2)

Table 4.1.3: The direct ionization cross section (in units of 10^{-16} cm^2) for positron impact on atomic hydrogen. The estimated uncertainty on these values is ±25% (see also Fig. 4.1.3)

E_0 (eV)	Recommended Direct Ionization Cross Section (x10^{-16} cm^2)
13.6	0
15	0.07
20	0.23
25	0.38
30	0.55
35	0.68
40	0.75
50	0.85
60	0.88
70	0.84
80	0.80
100	0.71
125	0.61
150	0.50
175	0.41
200	0.36
300	0.27
400	0.23
500	0.20
700	0.16

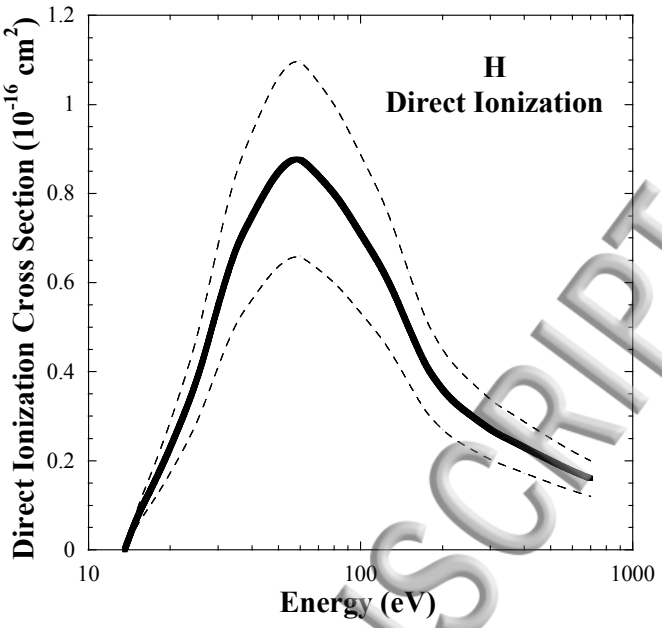

Figure 4.1.3. The recommended direct ionization cross section for positron impact on H - solid line. The dashed lines represent the estimated uncertainty limits of ±25% (see also Table 4.1.3)

4.2 Helium - He

In rather stark contrast to atomic hydrogen, helium (He) has perhaps been studied more than any other atomic system by low and intermediate energy positron scattering. An example of this are the more than 20 separate measurements of the total scattering cross section for He [157-179] spanning the period from the early 1970's until the present. For the positronium formation cross section there are fewer independent measurements [25,177,180-186] and fewer still for electronic excitation [22,187-190] and direct ionization [25,189,191-194]. The various cross section determinations for total scattering, positronium formation, and direct ionization have recently been assessed by Chiari and Zecca [11], who also proposed "recommended cross sections" for these three processes, and we will draw heavily on their assessments in the following sections.

4.2.1 Total Scattering

Absolute total scattering measurements for positron interactions with helium have been measured extensively since the 1970's, with the bulk of measurements being completed before the turn of tis century. Comparisons of the various measurements can be found in a number of recent papers [eg. 11,176-179] and we will not repeat those here. We also note the recent recommended total cross section of Chiari and Zecca [11] which they obtained by averaging a number of the results from more recent determinations of the total cross section, whilst ruling out some others that were either too high or too low in magnitude. In our view another reasonable gauge of the appropriate magnitude of the cross section, particularly at energies below the Ps threshold at 17.8 eV, are the recent state-of-the-art theoretical calculations [e.g. 146,195,196-198] which have been shown to agree extremely well both amongst themselves, and with the most accurate measurements [e.g. 174,176,179].

We do not see any need to greatly alter the recommended cross section of Chiari and Zecca, with the possible exception of the low energy (below 1 eV) values where we believe the present theory is possibly more accurate than experiment - which is also limited to just a few measurements in this energy region. We suggest therefore that the cross section of [11] should be about 5% higher at energies below about 1 eV. Otherwise, the values that we recommend are those proposed by Chiari and Zecca. For completeness we provide our full recommended total cross section in Table 4.2.1 and it is shown in Figure 4.2.1, where the error bounds, which we conservatively assess to be ±10%, are also given. This is perhaps the most accurately known positron scattering cross section – a benchmark.

4.2.2 Positronium Formation

There have been a number of absolute measurements of the Ps formation cross section [25,177,180-186]. At energies between the Ps formation threshold (17.8 eV) and about 30 eV, the agreement between the experimental values, particularly the most recent measurements [177,186], is excellent. At the peak in the cross section (35-45 eV), and for energies out to energies of about 100 eV, there are significant differences (30-40%) between the various measured cross sections, making the selection of a recommended cross section difficult. However, we can also be guided, somewhat, in choosing a set of recommended values by the weight of recent theoretical calculations [e.g. 86,197,198] which tend to favour a lower energy, lower magnitude peak cross section for the Ps formation channel. As a result of these differences, our recommended cross section, which shows a peak value of around 0.45 $Å^2$ at

an energy in the region of 40-45 eV, has a conservatively estimated uncertainty of ±15%. These values are given in Table 4.2.2 and shown in Figure 4.2.2.

4.2.3 Electronic Excitation

There are only a few measurements of absolute cross sections for electronic excitation of the helium atom by positron impact. These include the earlier measurements of Coleman and colleagues [22,187], Sueoka and colleagues [188,189] and the most recent data of Caradonna *et al.* [190]. These measurements are for the discrete excitation of the 2^1S and 2^1P states of He and of the unresolved n=2 excitation. Caradonna and co-workers also used their trap-based technique to measure the total inelastic cross section for He which represents the sum of all inelastic events, including ionization, but not including Ps formation. The results of these investigations, including a comparison with past and contemporary theory, is given in [190]. The recommended cross sections for the 2^1S and 2^1P states are given in Table 4.2.3 and are illustrated in Figure 4.2.3. The estimated uncertainties are ±25%.

4.2.4 Direct Ionization

Direct ionization cross section measurements are available from a number of experimental approaches – as discussed in section 2.5. The interplay of direct ionization, total ionization and Ps formation (which also leads to ionization), has also been used in some cases to deduce either positronium formation or direct ionization cross sections by subtraction of one or the other from the total ionization measurements. The absolute direct ionization cross section for He has been measured a number of times since the first investigations in the mid 1980's [25,189,191-194], with the cross sections of [193,194] being renormalised by [186]. The ionization cross sections have been discussed extensively in the review articles of Laricchia and colleagues [17,26] and by Chiari and Zecca [11], the latter providing recommended cross section values and uncertainties.

The level of agreement between the various experimental cross sections, and a number of theoretical approaches (see for e.g. [17,146]) is generally very good at energies from threshold up to 500 eV or more, so we feel there is no need for us to further adjust the recommended cross section of Chiari and Zecca [11], which we reproduce in Table 4.2.4 and show in Figure 4.2.5. The estimated uncertainties on these values are ±20%.

Table 4.2.1: The total cross section (in units of 10^{-16} cm^2) for positron scattering from helium. The absolute error is estimated to be ±10% (see also Fig. 4.2.1)

Energy (eV)	Recommended TCS (x10^{-16} cm^2)	Energy (eV)	Recommended TCS (x10^{-16} cm^2)
0.10	0.38	6.0	0.127
0.20	0.29	7.0	0.139
0.30	0.23	8.0	0.150
0.40	0.185	9.0	0.160
0.50	0.155	10	0.168
0.60	0.133	15	0.196
0.70	0.115	20	0.275
0.80	0.102	30	0.721
0.90	0.092	40	1.03
1.0	0.083	50	1.14
1.5	0.060	60	1.18
2.0	0.058	70	1.19
3.0	0.078	80	1.17
4.0	0.097	90	1.13
5.0	0.113	100	1.07

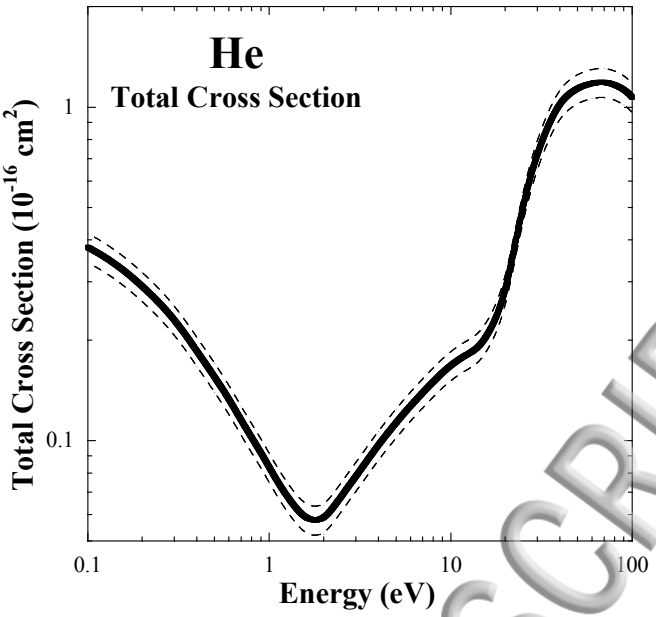

Figure 4.2.1. The recommended total positron scattering cross section for He (solid line), while the dashed lines represent the estimated uncertainty limits of ±10% (see also Table 4.2.1).

Table 4.2.2: The positronium formation cross section (in units of 10^{-16} cm^2) for helium. The absolute error is estimated to be ±15% (see also Fig. 4.2.2).

E (eV)	Recommended Positronium Formation Cross Section (x10^{-16} cm^2)	E (eV)	Recommended Positronium Formation Cross Section (x10^{-16} cm^2)
17.8	0	35	0.420
18.0	0.010	40	0.445
19.0	0.035	45	0.445
20	0.068	50	0.420
21	0.110	55	0.380
22	0.143	60	0.335
23	0.180	70	0.265
24	0.211	80	0.205
25	0.243	90	0.155
26	0.272	100	0.115
27	0.301	150	0.030
28	0.320		
29	0.345		
30	0.365		

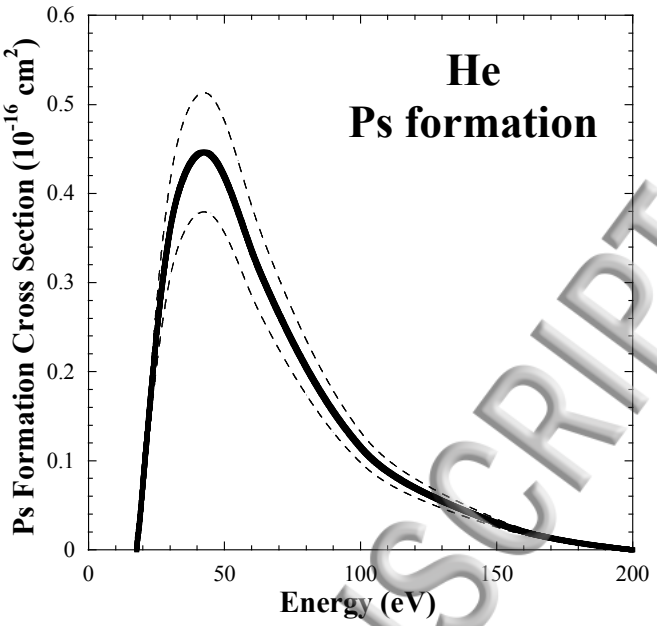

Figure 4.2.2. The recommended total positronium formation cross section for He - solid line. The dashed lines represent the estimated uncertainty limits of ±15% (see also Table 4.2.2).

Table 4.2.3: The cross section (in units of 10^{-16} cm^2) for positron impact excitation of the 2^1S and 2^1P states of He. The estimated uncertainty on these values is ±25% (see also Fig. 4.2.3 and 4.2.4)

E_0 (eV)	Recommended Cross Sections ($x10^{-16}$ cm^2)	
	2^1S	2^1P
20.6	0	-
21.0	0.003	-
21.2	-	0
22.0	0.011	0.0021
23.0	0.019	0.0066
24.0	0.027	0.0149
25.0	0.035	0.0232
26.0	0.042	0.0335
28.0	0.052	0.0522
30.0	0.058	0.0690
32	0.061	0.0833
34	0.062	0.094
36	0.060	0.103
38	0.057	0.109
40	0.054	0.112

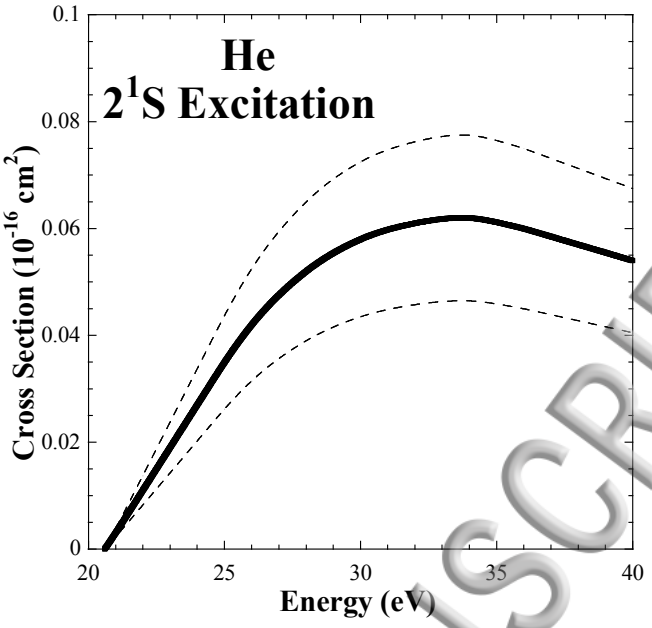

Figure 4.2.3. The recommended cross section for the excitation of He 2^1S - solid line. The dashed lines represent the estimated uncertainty limits of ±25% (see also Table 4.2.3)

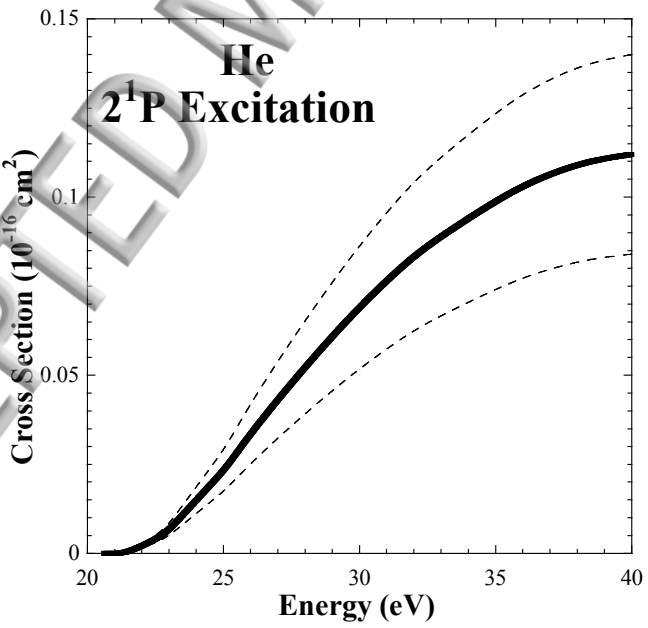

Figure 4.2.4. The recommended cross section for the excitation of He 2^1P - solid line. The dashed lines represent the estimated uncertainty limits of ±25% (see also Table 4.2.3).

Table 4.2.4: The direct ionization cross section (in units of 10^{-16} cm^2) for positron impact on helium. The estimated uncertainty on these values is ±20% (see also Fig. 4.2.5).

E_0 (eV)	Recommended Direct Ionization Cross Section ($x10^{-16}$ cm^2)
24.6	0
30	0.0215
40	0.124
50	0.255
60	0.369
70	0.450
80	0.500
90	0.528
100	0.540
150	0.506
200	0.446
300	0.351
400	0.281
500	0.229
600	0.196
700	0.169
800	0.149
900	0.136
1000	0.119

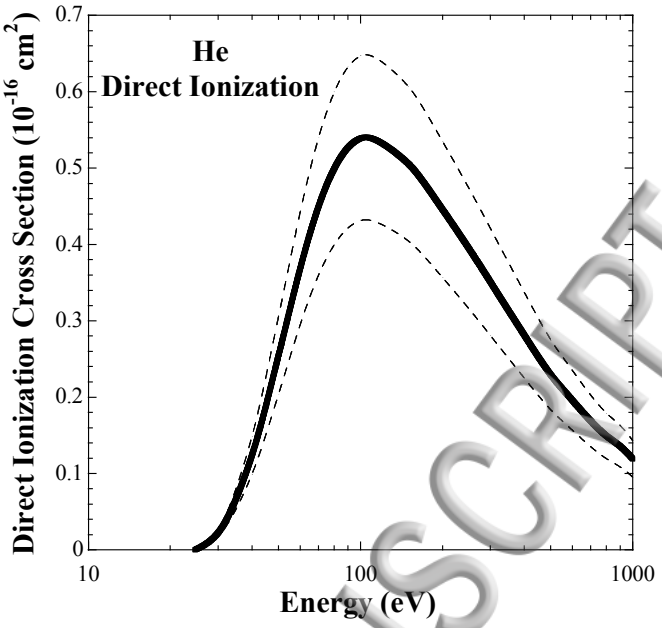

Figure 4.2.5. The recommended direct ionization cross section for positron impact on He - solid line. The dashed lines represent the estimated uncertainty limits of ±20% (see also Table 4.2.4).

4.3 Lithium - Li

4.3.1 Positronium Formation

To the best of our knowledge there is only one experimental investigation of positron scattering from lithium (Li) and that is a measurement of the positronium formation cross section by the Wayne State group [199]. They measured what they consider to be a "lower limit" on the Ps formation cross section by detecting the yield of two-gamma-ray coincidences arising from the decay of singlet positronium (see Section 2). Their measurements extend from 0.3 to 15.0 eV and we note that they only quote statistical uncertainties on the measurements. We further note that with a direct ionization threshold of 5.39 eV, the Ps formation channel for lithium is "open" at 0 eV.

We can also be guided in assessing a recommended cross section by a significant amount of theoretical activity for positron scattering by lithium [48,61,80,93,123]. As a "one-electron atom" with a large dipole polarisability, which arises principally from the resonant 2s-2p transition, the lithium atom lends itself to reasonably accurate treatment by contemporary theoretical calculations, particularly close-coupling approaches. The most recent of these approaches [61] is a convergent close coupling approach that also includes a two-centre expansion in the final state allowing, in principle, a more accurate treatment of the Ps formation cross section as well as for other scattering channels. A comparison of contemporary theory and the experiment of [199] can be found in [61]. In contrast to many other measurements of the Ps formation cross section, positronium formation appears to be essentially exhausted by about 30 eV, whereas in many other atoms and molecules it can still be significant above 50–100 eV. The recommended cross section, based on both experiment and theory, is given in Table 4.3.1 and shown in Figure 4.3.1. The estimated uncertainty is ±25%.

Table 4.3.1: The positronium formation cross section (in units of 10^{-16} cm^2) for lithium. The absolute error is estimated to be ±25% (see also Fig. 4.3.1).

E_0 (eV)	Recommended Positronium Formation Cross Section ($x10^{-16}$ cm^2)
0.1	19.6
0.2	28.7
0.3	34.2
0.5	39.2
0.8	41.9
1.0	42.1
1.5	41.4
2.0	38.7
3.0	33.3
4.0	27.0
5.0	20.8
7.5	12.5
10	8.2
15	3.5
20	1.8

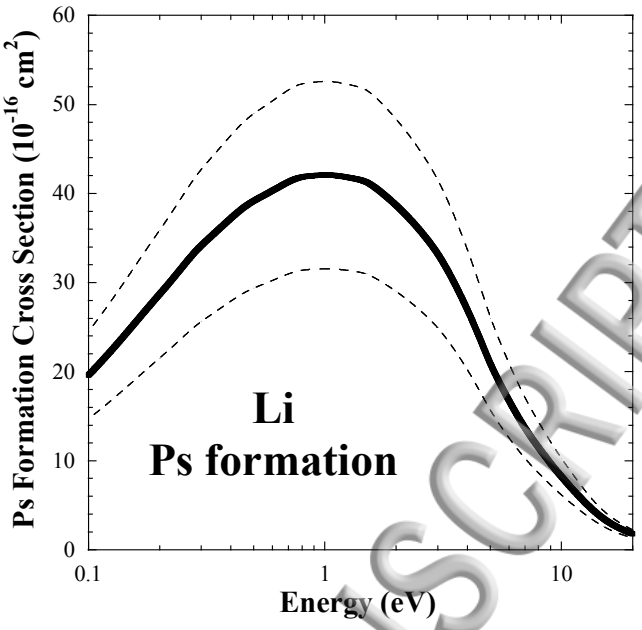

Figure 4.3.1. The recommended positronium formation cross section for Li - solid line. The dashed lines represent the estimated uncertainty limits of ±25% (see also Table 4.3.1).

4.4 Neon - Ne

There have been many studies of positron scattering from neon (Ne), with measurements of the total cross section [65,161,162,165,169-173,200-205], the positronium formation cross section [65,182,185,206-209], and the direct ionization cross section [26,189,191,192,208,210-213] having been reported. We also note several measurements [207,208,214] of the total ionisation cross section (direct ionization + positronium formation), and a measurement of the direct double ionization cross section [215]. There have also been a significant number of theoretical calculations of these various cross sections [65,97,100,126,129,197,216-233].

4.4.1 Total Scattering

The total scattering measurements and calculations have been discussed in some detail by Chiari and Zecca in their recent article [11]. They also provided a recommended total cross section based on what they perceived to be reasonably good agreement amongst the bulk of the (many) experimental measurements. We agree broadly with the rationale they have proposed, and also with the cross section they recommend and, as there have not been further measurements since this recommended data was published, we see no reason to add further to this. There has, however, been an additional, and detailed, many-body-theory calculation by Gribakin and colleagues [129], which is also broadly in agreement with the recommended cross section.

The recommended total positron scattering cross section for neon is given in Table 4.4.1 and shown in Figure 4.4.1. The estimated uncertainty on these cross section values is ±10%.

4.4.2 Positronium Formation

There have been a number of measurements of positronium formation in neon dating back to the early 1980's. The early results [182,206] appear to be superseded by higher quality results from the past 15 years [65,208,209]. These results, and contemporary theory, were compared and discussed by Chairi and Zecca in their review [11] but they did not assign a "recommended" cross section for Ps formation in Ne. The level of agreement between the three most recent measurements is reasonably good across the whole energy range from threshold to 200 eV, although the best agreement is found in the near-threshold region.

The recommended positronium formation cross section for neon is given in Table 4.4.2 and shown in Figure 4.4.2. The estimated uncertainty on these cross section values is ±15%.

4.4.3 Direct Ionization

The direct ionization cross section for neon has been reviewed in the work of Laricchia *et al* [26] and also recently assessed by Chiari and Zecca [11], but the latter chose not to provide a recommended cross section, most likely because the spread in the available experimental data is quite large, particularly in the vicinity of the cross section peak at around 150 eV. On the other hand, the level of agreement between the various experiments, and theory, between threshold (21.56 eV) and about 100 eV is reasonably good, the main exception to this being the earliest result of [191], which is larger in magnitude than all other results.

There are also several measurements of the total ionization cross section, but rather than analyse these, a recommended total ionization cross section could be obtained by adding the Ps formation and direct ionization cross sections.

The recommended direct ionization cross section for neon is given in Table 4.4.3 and shown in Figure 4.4.3. The estimated uncertainty on these cross section values is ±25%.

Table 4.4.1: The total cross section (in units of 10^{-16} cm^2) for positron scattering from neon. The estimated uncertainty is ±10% (see also Fig. 4.4.1).

Energy (eV)	Recommended TCS (x10^{-16} cm^2)	Energy (eV)	Recommended TCS (x10^{-16} cm^2)
0.25	0.274	7.0	0.752
0.30	0.229	8.0	0.784
0.40	0.180	9.0	0.809
0.50	0.164	10	0.831
0.60	0.155	15	1.04
0.70	0.156	20	1.40
0.80	0.161	30	1.71
0.90	0.170	40	1.87
1.0	0.184	50	1.90
1.5	0.265	60	1.94
2.0	0.329	70	1.95
3.0	0.466	80	1.95
4.0	0.569	90	1.95
5.0	0.651	100	1.91
6.0	0.710		

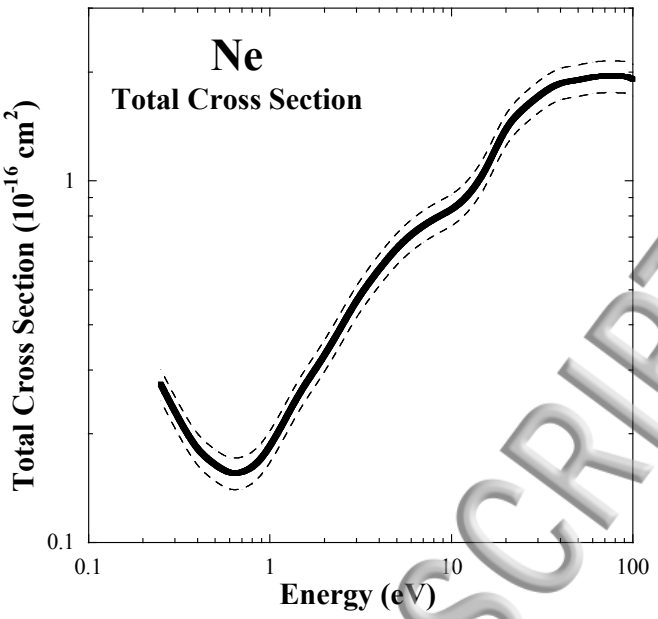

Figure 4.4.1. The recommended total positron scattering cross section for Ne (solid line), while the dashed lines represent the estimated uncertainty limits of ±10% (see also Table 4.4.1)

Table 4.4.2: The positronium formation cross section (in units of 10^{-16} cm^2) for neon. The estimated uncertainty is ±15% (see also Fig. 4.4.2).

E (eV)	Recommended Positronium Formation Cross Section (x10^{-16} cm^2)	E (eV)	Recommended Positronium Formation Cross Section (x10^{-16} cm^2)
14.76	0	40	0.45
15.0	0.09	50	0.38
16.0	0.17	60	0.33
17.0	0.23	70	0.27
18.0	0.28	80	0.23
20	0.38	90	0.20
22	0.44	100	0.17
24	0.47	125	0.10
26	0.49	150	0.055
28	0.50	175	0.018
30	0.50		
32	0.49		
35	0.48		

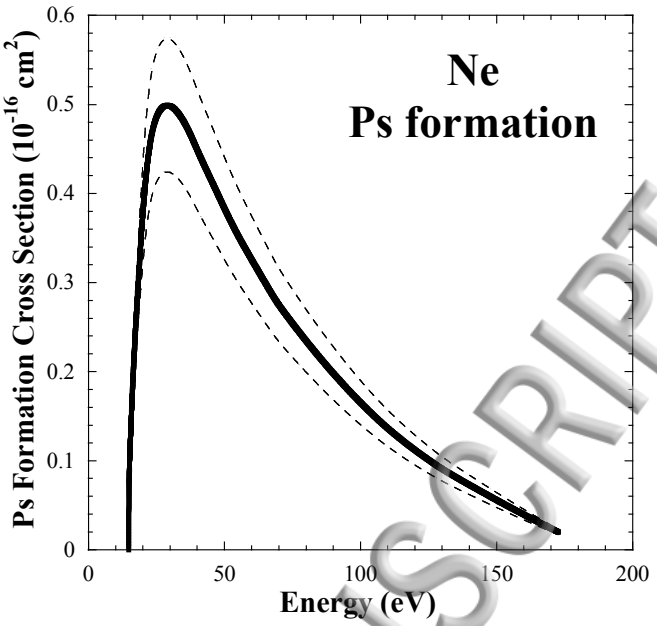

Figure 4.4.2. The recommended positronium formation cross section for Ne - solid line. The dashed lines represent the estimated uncertainty limits of ±15% (see also Table 4.4.2).

Table 4.4.3: The direct ionization cross section (in units of 10^{-16} cm^2) for positron impact on neon. The estimated uncertainty on these values is ±25% (see also Fig. 4.4.3).

E_0 (eV)	Recommended Direct Ionization Cross Section (x10^{-16} cm^2)
21.6	0
25	0.042
30	0.113
40	0.275
50	0.40
75	0.65
100	0.77
125	0.80
150	0.79
200	0.75
300	0.67
500	0.53
750	0.39
1000	0.30

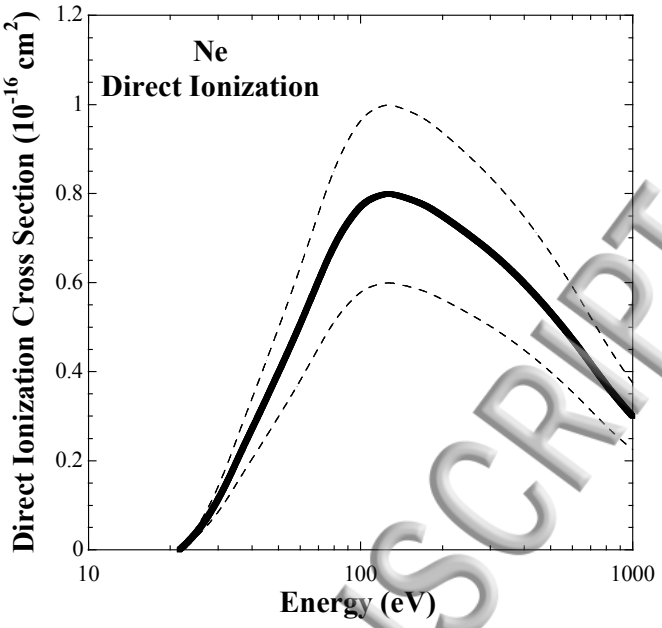

Figure 4.4.3. The recommended direct ionization cross section for positron impact on Ne - solid line. The dashed lines represent the estimated uncertainty limits of ±25% (see also Table 4.4.3).

4.5 Sodium - Na

Experimental measurements of positron scattering by sodium (Na) are rather few, with the only processes studied being total scattering [234,235] and positronium formation [236,199], and these studies all emanated from the Wayne State group. There have, however, been a number of theoretical calculations of positron-alkali interactions (e.g. [41,48,54,95,123,237-239]) and, as was the case with lithium, we can expect a reasonable level of accuracy from these given the 'one-electron' nature of the target.

4.5.1 Total Scattering

Total scattering measurements have been made in the energy range from 3-102 eV [234] and 1-10 eV [235], both experiments using the attenuation method and the Beer-Lambert law to obtain absolute cross sections. These authors discuss the potential effects of their inability to discriminate between unscattered particles and forward elastically scattered positrons, an effect which renders the measured cross section lower than the true value (see e.g. [20]). These effects were estimated to be as large as 40% at the lowest energy, reducing to around 3% at 50 eV. Some effort was made [41,48] to calculate 'effective' total cross sections using differential scattering cross sections from theory to estimate the forward scattering correction. In general, the agreement between the (adjusted) experimental values and calculations is reasonably good across the measured energy range. The recommended total positron-sodium scattering cross section is presented in Table 4.5.1 and shown in Figure 4.5.1. The estimated absolute uncertainty on these values is 20%, which is possibly a little conservative at the higher energies.

4.5.2 Positronium Formation

To the best of our knowledge there have only been two measurements of Ps formation for sodium, both by the Wayne State group [236,199], and these are for energies between 1.5 and 10 eV. These are largely in agreement with each other, within experimental uncertainty, and agree well with state-of-the-art theory for energies greater than about 1 eV. However the most recent experimental determination [199] shows a completely different energy dependence to theory below about 1 eV, with that experiment continuing to rise to a value in excess of 80 $Å^2$ at 0.15 eV, while theory decreases in magnitude at energies lower than 1 eV. Indeed, three independent close coupling calculations show a maximum value of around 25 $Å^2$ at 1.5 eV [237,238,123]. This smaller, low energy cross section has also been confirmed recently by a two-centre, convergent close-coupling calculation [239]. As a result we (cautiously) favour a smaller Ps formation cross section at low energies, but also strongly suggest further experimental work is required in this energy range below about 3 eV. We also note that this decreasing cross section at low energies is consistent with what is observed in both experiment and theory for Li and K atoms.

The recommended Ps formation cross section for sodium is given in Table 4.5.2 and shown in Figure 4.5.2., with the recommended uncertainty on the cross section being 30%.

Table 4.5.1: The total cross section (in units of 10^{-16} cm^2) for positron scattering from sodium. The estimated uncertainty on these values is ±20% (see also Fig. 4.5.1).

E_0 (eV)	Recommended TCS (x10^{-16} cm^2)
1.0	140
3.0	102
5.0	86
7.0	77
10	67
20	50
30	40
50	29
75	21
100	16

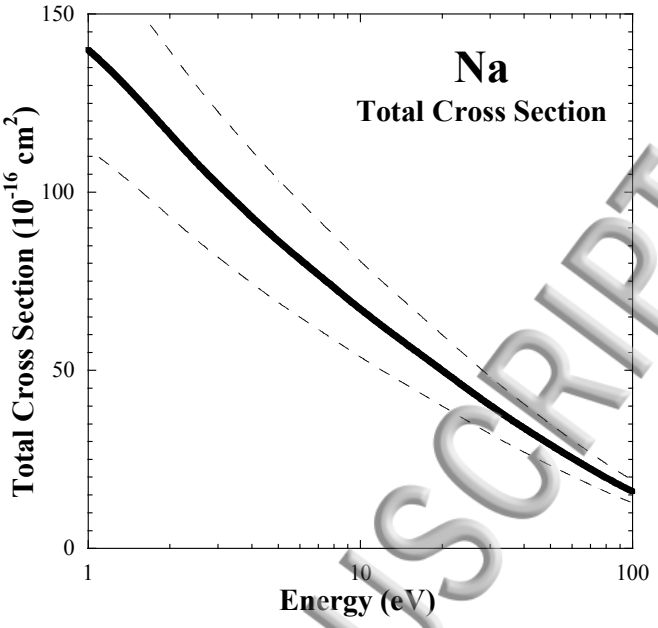

Figure 4.5.1. The recommended total cross section for positron scattering from Na - solid line. The dashed lines represent the estimated uncertainty limits of ±20% (see also Table 4.5.1).

Table 4.5.2: The positronium formation cross section (in units of 10^{-16} cm^2) for sodium. The estimated uncertainty on these values is ±30% (see also Fig. 4.5.2).

E_0 (eV)	Recommended Positronium Formation Cross Section ($x10^{-16}$ cm^2)
0.15	25
0.50	30
1.0	36
1.5	39
2.0	40
3.0	37
5.0	28
10	15
20	5

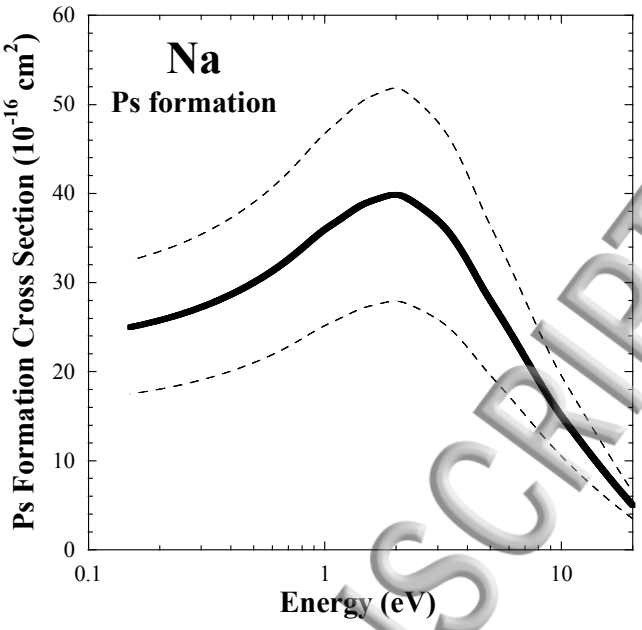

Figure 4.5.2. The recommended positronium formation cross section for Na - solid line. The dashed lines represent the estimated uncertainty limits of ±30% (see also Table 4.5.2).

4.6 Magnesium - Mg

There are only a few experimental measurements of positron scattering from magnesium, which have been conducted by the Wayne State group [240,149,241], and involved the measurement of the total scattering cross section and the Ps formation cross section. To our knowledge there are no measurements of the direct ionization cross section. There have also been a number of theoretical calculations which have provided comparison to the experimental work [63,85,242-250].

4.6.1 Total Scattering

Total scattering measurements have been made in the energy range from about 3-60 eV [240,149], with the latter measurement representing the final determination of this cross section by the Wayne State group. There have also been a number of theoretical investigations and, indeed, one of the significant and outstanding issues, at least experimentally, is the prediction by theory of a very large p-wave shape resonance in the elastic scattering cross section at low energies. While there are some small differences in the position and magnitude of this resonance, recent, accurate theoretical calculations [247-250] all agree as to the existence of this feature and, if confirmed, it would represent one of the largest scattering resonances in either electron or positron scattering – an interesting outcome given the otherwise complete (detected) absence of positron scattering resonances in most atomic and molecular scattering systems.

Given this interest the recommended total cross section we provide is a combination of both experiment and theory as we feel it is significant to highlight the existence of this resonance and its enormous, predicted magnitude. Hopefully this will also provide stimulus for further experimentation.

The recommended cross section is shown in figure 4.6.1. That part of the cross section based on experiment and theory is shown as the thick solid line, while that based on theory alone (below 2 eV) as the thick dashed line. The thin dashed lines represent the estimated uncertainty at ±20%.

4.6.2 Positronium Formation

There has only been one experimental measurement of the Ps formation cross section for magnesium [241], and the authors claim this to be a preliminary result. It actually comprises two measured cross sections – an "upper level" based on measurements of transmitted positron intensities, and a "lower level" estimate based on measurements of decay gamma rays. These differ in places by a factor of three and, while there are several sophisticated theoretical calculations available for comparison [243,244,246,63], they also show a significant variation in the predicted cross section values. A comparison of the experiment and theory can be found in the recent paper of Utamuratov et al. [63].

Accordingly we do not provide a "recommended" cross section for Ps formation in Mg and note that further experimental work would be useful.

Table 4.6.1: The total cross section (in units of 10^{-16} cm^2) for positron scattering from Mg. A conservative estimate of the absolute error is ±20% (see also Fig. 4.6.1).

E_0 (eV)	Recommended TCS (x10^{-16} cm^2)
0.01	265
0.05	391
0.1	971
0.15	1007
0.2	836
0.5	358
1	229
2	161.2
5	96.7
10	61.0
15	47.5
20	39.2
30	31.5
40	26.6
50	23.2

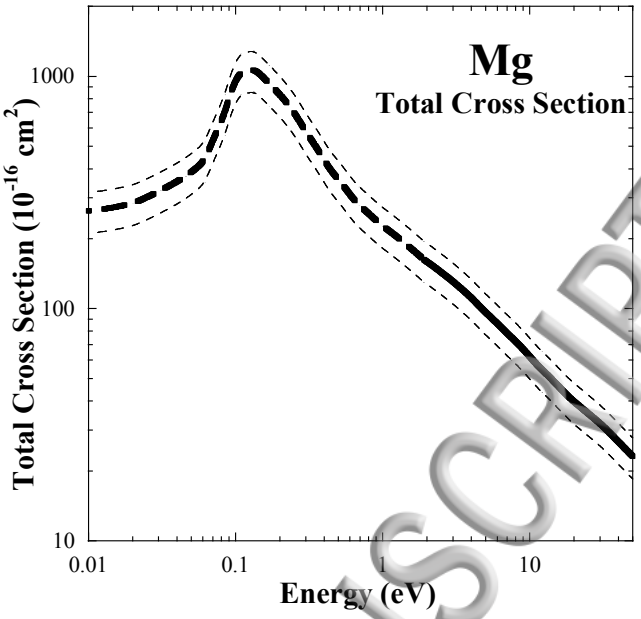

Figure 4.6.1. The recommended total cross section for positron scattering from Mg. The solid line is based on both experiment and theory while the thick dashed lines is based on theory alone (see text). The thin dashed lines represent the estimated uncertainty limits of ±20% (see also Table 4.6.1).

4.7 Argon - Ar

Positron scattering from argon (Ar) has possibly received more experimental and theoretical attention than any of the other heavy rare gas atoms, no doubt due to the ready availability and use of argon as a target gas. There have been a large number of total scattering cross section measurements [65,161,162,165,171-173,200-202,204,251-254], as well as measurements of the positronium formation cross section [65,181,182,185,207-209,236,255-258], electronic excitation [8] and the direct ionization cross section [189,191-193,210,211,213]. There have also been a considerable number of theoretical calculations of these various processes [65,97,100,126,128,129,197,216,218,221-227,229-233,259-265]. We also note a previous cross section set for argon [108] which was developed to aid the modeling of positron transport in argon, but tabulated values were not presented.

4.7.1 Total Scattering

Total scattering cross sections have been measured extensively and, of all the rare gas atoms, the level of difference between the measurements for argon is probably the greatest. This is particularly the case at low energies, where there are differences in magnitude between some of the measured cross sections of between 50-100% at energies between 1 and 10 eV. It has been demonstrated that much of this difference in magnitude could be due to the effects of forward scattering [20].

Chiari and Zecca [11] have recently reviewed the various total cross section measurements and have proposed a recommended cross section for argon. We are largely in agreement with their assessment of the available data, with the exception of the magnitude of the cross section at the lowest energies. Below 1 eV there are only a few reliable measurements but, more recently, accurate theoretical approaches have emerged [e.g. 58,61] which predict a smaller cross section at lower energies.

Thus our recommended total cross section is identical to that of Chiari and Zecca above 1 eV, but slightly lower in magnitude between 0.1–1.0 eV. The recommended values are given in Table 4.7.1 and shown in Figure 4.7.1. The estimated uncertainty on these cross section values is ±10%.

4.7.2 Positronium Formation

The positronium formation cross section was also reviewed by Chiari and Zecca, but they declined to propose a recommended cross section for this process in argon. With a few possible exceptions, the level of agreement between the various measurements of the Ps formation cross section is reasonably good. The most significant level of disagreement between recent measurements (~20%) occurs in the region of the cross section maximum between about 15 and 40 eV. Most of the earlier measurements from the 1980's and 90's are larger in magnitude across the whole energy range than the more recent studies, and the weight of theoretical work also favours a lower magnitude cross section across the whole energy range.

Our recommended positronium formation cross section is given in Table 4.7.2 and shown in figure 4.7.2. The estimated uncertainty on the cross section values is ±15%.

4.7.3 Electronic Excitation

There has been one measurement of electronic excitation in argon by positron impact [8] by the San Diego group. They measured the total excitation cross section for the components of the $3p^5$ 4s manifold in argon with total angular momentum J=1 – namely the $3p^5(^2P_{3/2,1/2})4s$ levels from near threshold (11.63 eV) to 30 eV. We summarise their results here by suggesting a recommended cross section for the two combined excited states, noting their data shows the cross section for the 1/2 level to be about a factor of 3-4 larger than that for the 3/2 level.

The recommended cross section for the $3p^5$ 4s excitation in argon is given in Table 4.7.3 and shown in Figure 4.7.3. The estimated uncertainty is ±15%.

4.7.4 Direct Ionization

The direct ionization cross section has been measured by several groups [189,191-193,210,211,213], and has been discussed recently by Chiari and Zecca [11] and Laricchia and colleagues [26], and the level of agreement between experimental measurements is relatively high. With the exception of one of the earlier measurements of direct ionization [191], which resulted in a much higher cross section, most of the measurements and theory are in agreement across the whole energy range, from threshold (15.75 eV) to 1000 eV, to within about 20%.

The recommended direct ionization cross section is given in Table 4.7.4 and shown in figure 4.7.4. The estimated uncertainty on these values is ±15%.

Table 4.7.1: The total cross section (in units of 10^{-16} cm^2) for positron scattering from argon. The estimated uncertainty is ±10% (see also Fig. 4.7.1).

Energy (eV)	Recommended TCS (x10^{-16} cm^2)	Energy (eV)	Recommended TCS (x10^{-16} cm^2)
0.3	13.0	8	3.73
0.4	10.5	9	4.12
0.5	9.00	10	4.70
0.6	7.90	15	6.38
0.7	6.70	20	6.58
0.8	6.10	30	7.07
0.9	5.40	40	7.28
1.0	4.90	50	7.14
1.5	3.94	60	7.02
2	3.91	70	6.90
3	3.82	80	6.68
4	3.75	90	6.42
5	3.72	100	6.20
6	3.66		
7	3.64		

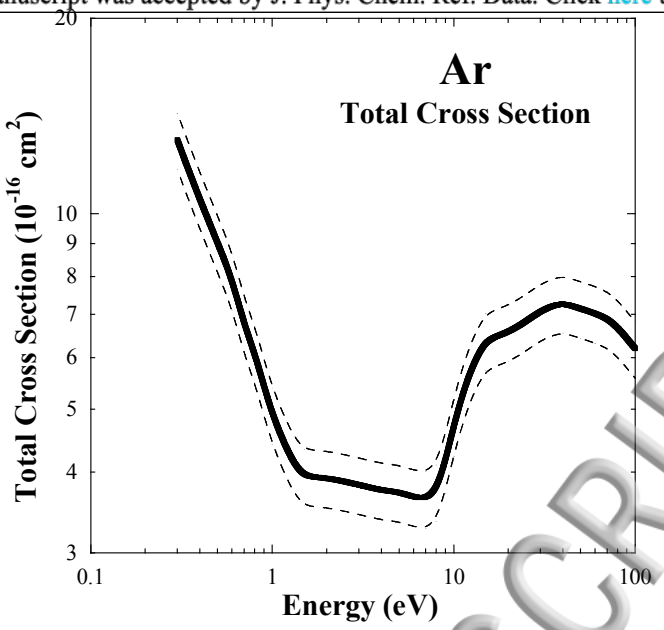

Figure 4.7.1. The recommended total positron scattering cross section for Ar (solid line), while the dashed lines represent the estimated uncertainty limits of ±10% (see also Table 4.7.1).

Table 4.7.2: The positronium formation cross section (in units of 10^{-16} cm^2) for argon. The estimated uncertainty is ±15% (see also Table 4.7.2).

E (eV)	Recommended Positronium Formation Cross Section (x10^{-16} cm^2)	E (eV)	Recommended Positronium Formation Cross Section (x10^{-16} cm^2)
8.95	0	25	2.65
10	0.95	30	2.53
11	1.47	40	2.23
12	1.93	50	1.75
13	2.26	60	1.32
14	2.52	70	0.98
15	2.68	80	0.68
16	2.77	90	0.46
17	2.80	100	0.29
18	2.79	125	0.05
19	2.78		
20	2.76		

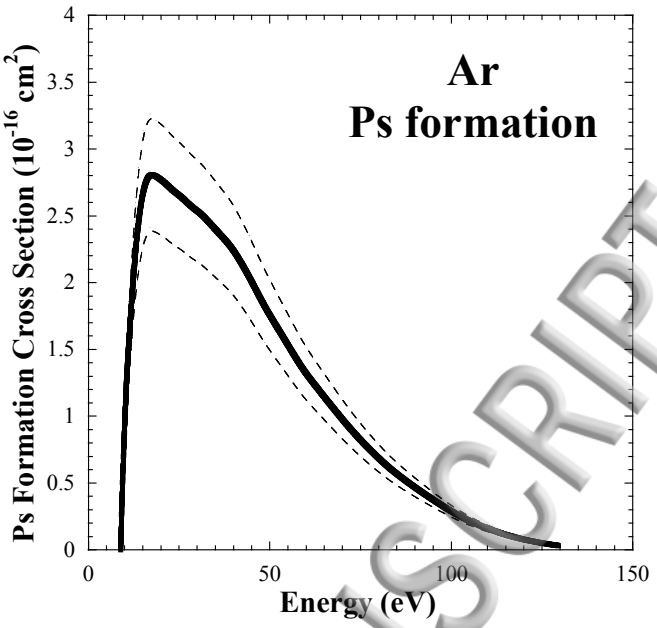

Figure 4.7.2. The recommended positronium formation cross section for Ar - solid line. The dashed lines represent the estimated uncertainty limits of ±15% (see also Table 4.7.2).

Table 4.7.3: The cross section for positron impact excitation of the $3p^5$ 4s levels in argon (in units of 10^{-16} cm^2). The estimated uncertainty on these values is ±15% (see also Fig. 4.7.3.).

E_0 (eV)	Recommended Excitation Cross Section ($x10^{-16}$ cm^2)
12	0.112
13	0.39
14	0.49
15	0.40
16	0.43
18	0.35
20	0.36
22.5	0.37
25	0.51
27.5	0.53
30	0.58

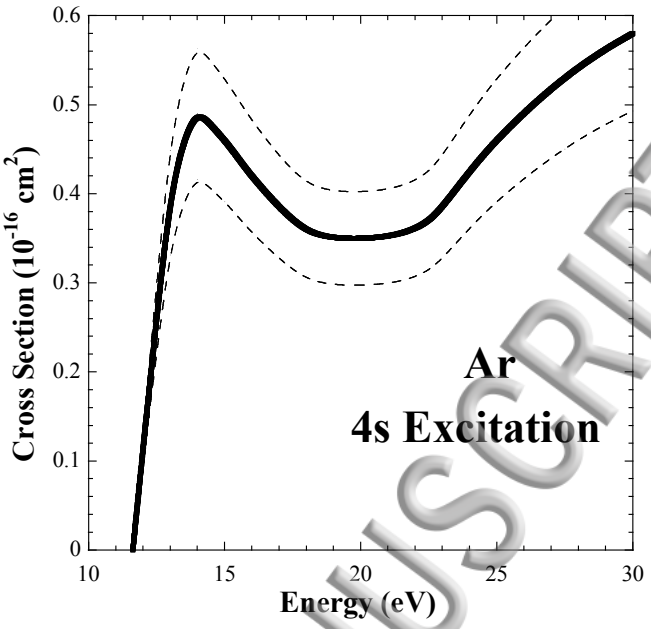

Figure 4.7.3: The cross section for positron impact excitation of the $3p^5$ 4s levels in argon - solid line. The dashed lines represent the estimated uncertainty limits of ±15% (see also Table 4.7.3).

Table 4.7.4: The direct ionization cross section (in units of 10^{-16} cm^2) for positron impact on argon. The estimated uncertainty on these values is ±15% (see also Fig. 4.7.4).

E_0 (eV)	Recommended Direct Ionization Cross Section (x10^{-16} cm^2)
15.75	0
20	0.26
30	0.99
50	2.31
75	2.83
100	2.96
150	2.77
200	2.46
300	1.95
400	1.58
500	1.34
750	0.91
1000	0.64

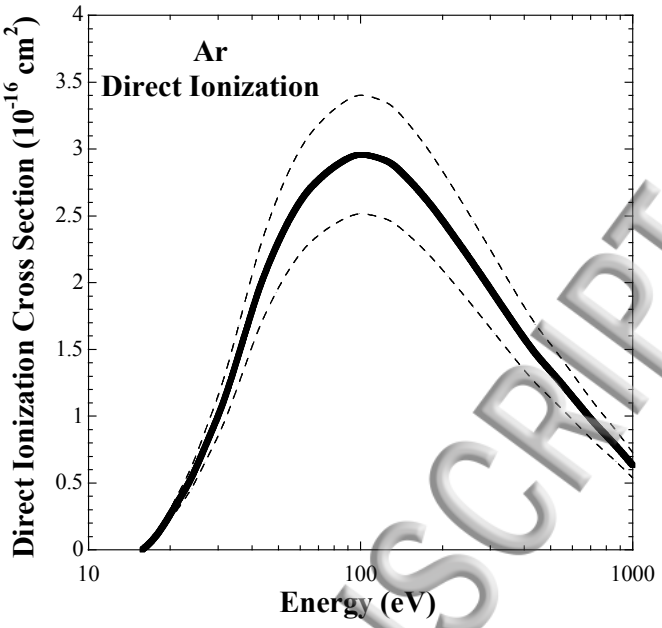

Figure 4.7.4. The recommended total direct ionization cross section for positron impact on Ar - solid line. The dashed lines represent the estimated uncertainty limits of ±15% (see also Table 4.7.4).

4.8 Potassium - K

Investigations of positron scattering from potassium (K) consist of just three experimental studies and again, they are all by the Wayne State group. The total scattering cross section has been measured by Kwan et al. [234] at energies between 8 and 98 eV and by Parikh et al. [266] from 1 to 102 eV. Positronium formation has been studied by Zhou et al. [236] at energies between 1 and 100 eV. There have also been a number of theoretical calculations of both the total scattering and the Ps formation cross sections [41,43,48,81,84,92,267].

4.8.1 Total Scattering

The measured total scattering cross section for potassium [234,266] shows similar behaviour as a function of energy as that for lithium – it exhibits a large, low energy peak (110 $Å^2$ at around 10 eV) before decreasing in magnitude at both higher and lower energies. We note that due to angular discrimination issues in the experiment, the measured cross section at low energies likely underestimates the true value by a considerable amount. This has been discussed previously, and indeed Kwan et al. [234] indicate in their manuscript that this effect may as large as 14% at 10 eV, reducing to 2% at 50 eV. They place an estimated absolute uncertainty on their cross sections of 21%, not including the possibility of forward scattering effects. Two close coupling calculations [81,92], both of which include elastic scattering and excitation of a number of bound states, as well as Ps formation, reveal a total cross section which is in good agreement with the experiment, but only if the experimental values are scaled upwards by a factor of 1.1, and further corrected at low energies for forward scattering effects (see for example figure 7 of [92]). Doing so moves the cross section peak closer to 150 $Å^2$ in magnitude.

Our recommended total cross section for positron scattering from potassium is given in table 4.8.1 and shown in figure 4.8.1. The estimated uncertainty is 20%.

4.8.2 Positronium Formation

The measured positronium formation cross section [236] consists of both upper and lower limit estimates, as discussed previously in Section 2. The difference between these estimates is significant (about a factor of three) at low energies and it appears that modern theory clearly favours the energy dependence and magnitude of the lower limit measurement [see e.g. 81,92]. Given the expected accuracy of these multi-configuration close coupling calculations for one-electron systems, even for the difficult Ps formation cross section, we are inclined to also favour the lower limit measurement for this cross section.

The recommended Ps formation cross section is given in Table 4.8.2 and shown in figure 4.8.2. The estimated uncertainty is ±30%.

Table 4.8.1: The total cross section (in units of 10^{-16} cm^2) for positron scattering from potassium. The estimated uncertainty is ±20% (see also Fig. 4.8.1).

E_0 (eV)	Recommended TCS (x10^{-16} cm^2)
1.0	100
2.5	120
5.0	162
8.0	157
10	142
15	111
20	92
30	72
45	57
60	47
80	37
100	30

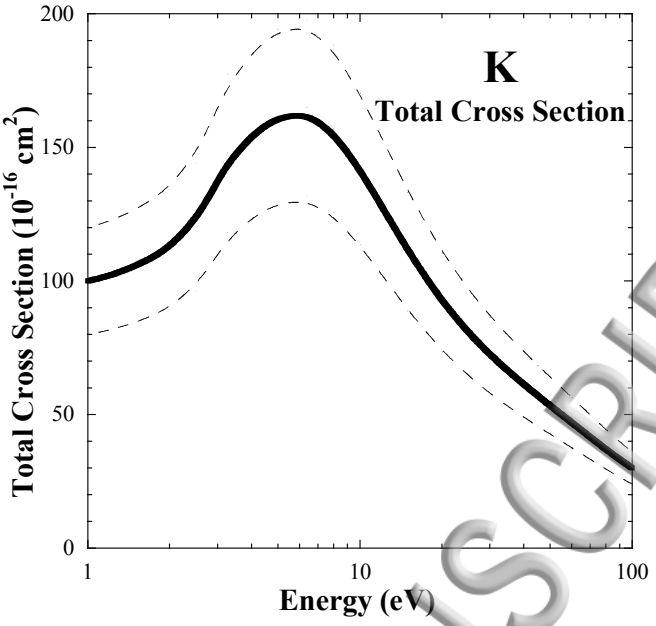

Figure 4.8.1. The recommended total cross section for positron scattering from K - solid line. The dashed lines represent the estimated uncertainty limits of ±20% (see also Table 4.8.1).

Table 4.8.2: The positronium formation cross section (in units of 10^{-16} cm^2) for potassium. The estimated uncertainty is ±30% (see also Fig. 4.8.2).

E_0 (eV)	Recommended Positronium Formation Cross Section ($x10^{-16}$ cm^2)
1.0	10
1.5	16.7
2.0	21
3.0	27
5.0	34
7.5	31
10	23.8
15	14.5
30	5.4
50	2.2
100	1.3

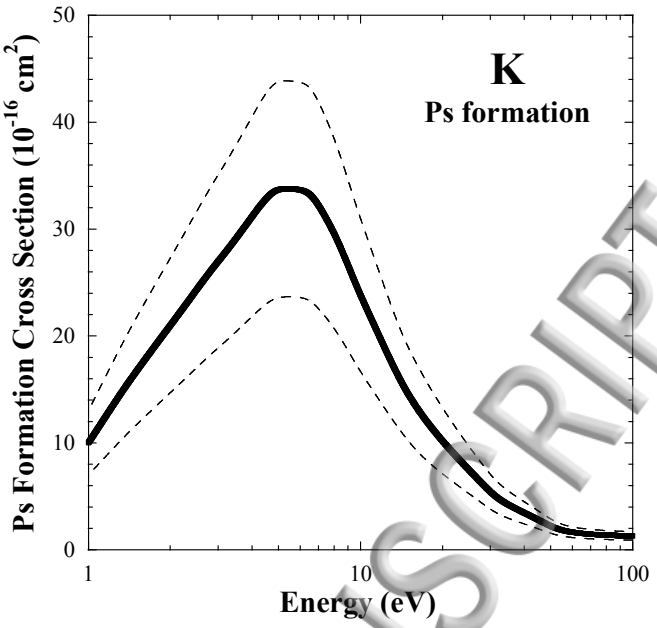

Figure 4.8.2. The recommended positronium formation cross section for K - solid line. The dashed lines represent the estimated uncertainty limits of ±30% (see also Table 4.8.2).

4.9 Krypton - Kr

There have been measurements of the total scattering [67,161,162,172,179,268-271], positronium formation [67,149,182,185,208,209,272] and direct ionization [193,209,212,213] cross sections for positron impact on krypton (Kr). There have also been numerous theoretical calculations of these various processes [67,97,100,126-129,197,216,223,224,227,229,230,232,233,264,265,273-275].

4.9.1 Total Scattering

Total cross section (TCS) measurements for positron scattering from krypton date back to the 1970's and there have been a reasonable number of subsequent experimental determinations since then [67,161,162,172,179,268-271]. The level of agreement between these experiments is mixed, with several apparently suffering from the effects of insufficient discrimination against forward scattering, which results in an anomalously low cross section, particularly at low energies.

Chiari and Zecca [11] have recently reviewed the available TCS data and have proposed a recommended TCS based on their analysis, and a comparison with theoretical predictions. Since their work there have been two other relevant determinations of this cross section, one experimental [179], and one theoretical [129], and these are also consistent with the recommended values. Indeed the latter calculation indicates that the low energy cross section recommended by Chiari and Zecca, which they speculated may be too low in magnitude, may in fact be a reasonable estimate.

Thus our recommended total cross section is identical to that of Chiari and Zecca. The recommended values are given in Table 4.9.1 and shown in Figure 4.9.1. The estimated uncertainty on these cross section values is ±10%.

4.9.2 Positronium Formation

There have been a number of measurements of the Ps formation cross section for Kr [67,149,182,185,208,209,272] and, as was the case in some of the lighter rare gases, the only significant discrepancies between these measurements occurs in the energy region around the peak in the cross section, at around 15-20 eV, where there are differences between the various measurements of up to 20%. Chiari and Zecca discussed these measurements but declined to recommend a Ps formation cross section. The various theoretical calculations for this process also show similar, if not larger, differences in this energy range. On the other hand, the agreement between experiments at near-threshold and higher energies is reasonably good.

Our recommended positronium formation cross section is given in Table 4.9.2 and shown in Figure 4.9.2. The estimated uncertainty on the cross section values is ±15%.

4.9.3 Direct Ionization

There are only a few experimental measurements of the direct ionization cross section by positron impact on krypton, with the majority from the UCL group [193,212,213] and one determination from the UCSD group [209]. The agreement between these cross sections is rather good in the near-threshold region but, once again, the measurements diverge somewhat

in the region from about 50 eV up to the cross section maximum at around 100 eV. At the maximum, the UCSD group predicts a cross section that is about 20% higher than that of the UCL group [213]. The only available data above 100 eV is that of the UCL group and this indicates a finite ionization cross section out to energies above 1000 eV.

These cross sections were also analysed by Chiari and Zecca [11] and Laricchia and colleagues [26], but they did not a suggest recommended cross section.

The recommended direct ionization cross section is given in Table 4.9.3 and shown in Figure 4.9.3. The estimated uncertainty on these values is ±20%.

Table 4.9.1: The total cross section (in units of 10^{-16} cm^2) for positron scattering from Kr. The estimated uncertainty on these values is ±10% (see also Fig. 4.9.1).

Energy (eV)	Recommended TCS (x10^{-16} cm^2)	Energy (eV)	Recommended TCS (x10^{-16} cm^2)
0.2	67.2	6	6.71
0.3	43.8	7	7.15
0.4	31.8	8	8.14
0.5	24.2	9	9.09
0.6	19.4	10	9.73
0.7	16.4	15	10.9
0.8	14.2	20	11.3
0.9	12.5	30	11.5
1.0	11.2	40	11.4
1.5	8.97	50	11.1
2	8.32	60	10.9
3	7.67		
4	7.23		
5	6.88		

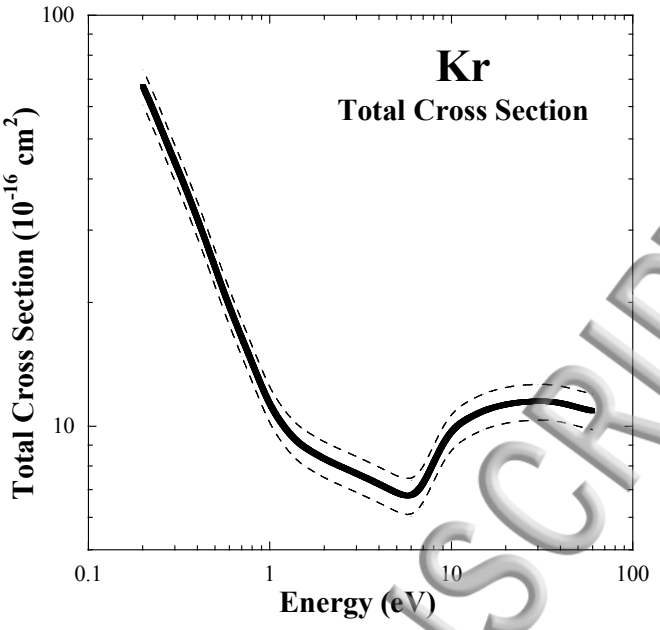

Figure 4.9.1. The recommended total positron scattering cross section for Kr (solid line), while the dashed lines represent the estimated uncertainty limits of ±10% (see also Table 4.9.1).

Table 4.9.2: The positronium formation cross section (in units of 10^{-16} cm^2) for Kr. The estimated uncertainty on these values is ±15% (see also Fig. 4.9.2).

E (eV)	Recommended Positronium Formation Cross Section (x10^{-16} cm^2)	E (eV)	Recommended Positronium Formation Cross Section (x10^{-16} cm^2)
7.2	0	25	3.76
7.5	0.70	30	3.37
8	1.50	40	2.61
9	2.58	50	2.06
10	3.30	60	1.58
11	3.82	70	1.17
12	4.24	80	0.82
13	4.45	90	0.56
14	4.55	100	0.37
15	4.56	125	0.04
16	4.55		
18	4.38		
20	4.21		

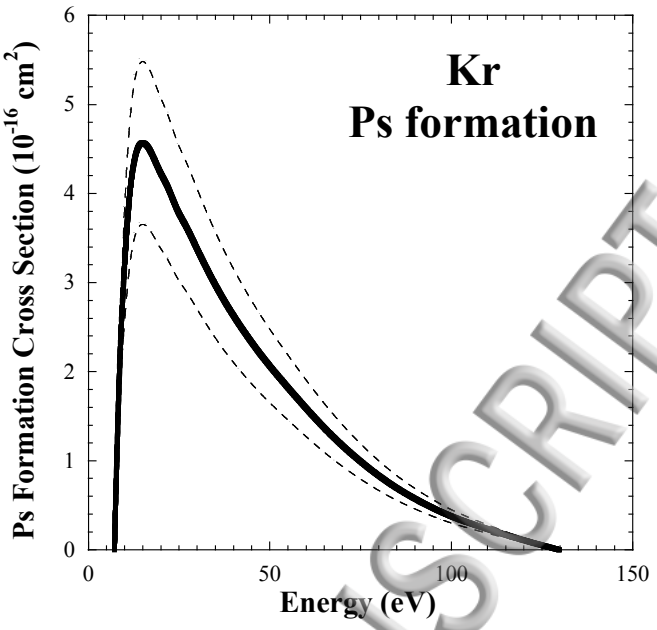

Figure 4.9.2. The recommended positronium formation cross section for Kr - solid line. The dashed lines represent the estimated uncertainty limits of ±15% (see also Table 4.9.2).

Table 4.9.3: The direct ionization cross section (in units of 10^{-16} cm^2) for positron impact on krypton. The estimated uncertainty on these values is ±20% (see also Fig. 4.9.3).

E_0 (eV)	Recommended Direct Ionization Cross Section ($x10^{-16}$ cm^2)
14	0
16	0.11
18	0.25
20	0.48
25	1.21
30	1.88
40	2.92
50	3.66
75	4.24
100	4.22
125	3.94
150	3.61
200	3.04
500	1.54
750	1.17
1000	0.95

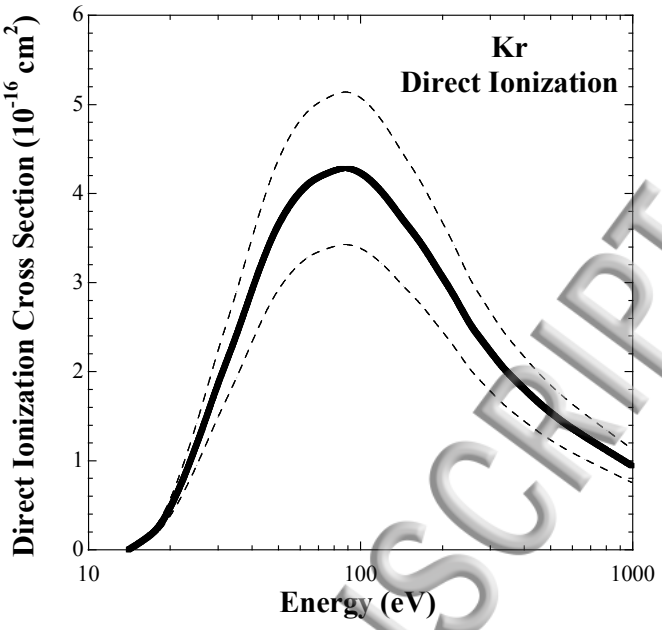

Figure 4.9.3. The recommended direct ionization cross section for positron impact on Kr - solid line. The dashed lines represent the estimated uncertainty limits of ±20% (see also Table 4.9.3).

4.10 Rubidium - Rb

There is only one measurement each of the total scattering cross section and positronium formation cross section for rubidium (Rb), and these are from the Wayne State group [266,276]. There are also a number of theoretical calculations of these cross sections [44,82,94,114,116,224,277] using a variety of techniques including the close coupling, Glauber, and polarised orbital approaches.

4.10.1 Total Scattering

The total scattering cross section has been measured between 1-100 eV [266]. The measurements, as for potassium, exhibit a strong cross section maximum at low energies, at around 5 eV in the case of Rb. Kernoghan *et al.* [94], performed close-coupling calculations for elastic scattering and excitation of Ps (1s, 2s, 2p, 3s, 3p and 3d) and Rb states (5s, 5p, 6s, 6p and 4d) and, by compiling these cross sections, also determined a total scattering cross section for Rb. A similar approach was more recently adopted by Chin *et al.* [82]. Kernoghan *et al.* also addressed the issue of forward angular discrimination in the experimental cross sections by using their differential elastic scattering cross sections to correct the experimental values for the experimentally estimated missing angular ranges [266] – 23° at 2 eV reducing to less than 9° above 30 eV. These corrected values, when scaled upward by a further 5%, were found to be in very good agreement with the calculated total cross section (see figure 5 of [94]).

Our recommended total cross section for positron scattering from rubidium is given in Table 4.10.1 and shown in Figure 4.10.1. The estimated uncertainty is 25%.

4.10.2 Positronium Formation

The positronium formation cross section has been measured by Surdutovich *et al.* [276] at energies between 1-17 eV. There have also been several calculations of the cross section for this channel (e.g. [82,94]), which is "open" and non-zero in magnitude at 0 eV. Both theory and experiment indicate a cross section which peaks near 5 eV in energy and with a magnitude around 40 $Å^2$, although there is a reasonable level of uncertainty around this value.

The recommended Ps formation cross section is given in Table 4.10.2 and shown in Figure 4.10.2. The estimated uncertainty is ±30%.

Table 4.10.1: The total cross section (in units of 10^{-16} cm^2) for positron scattering from rubidium. The estimated uncertainty in these values is ±25% (see also Fig. 4.10.1).

E_0 (eV)	Recommended TCS (x10^{-16} cm^2)
1.0	108
2.0	124
3.0	148
5.0	177
6.0	180
7.0	163
15	136
20	115
30	88.5
50	62.5
75	45.0
100	35.0

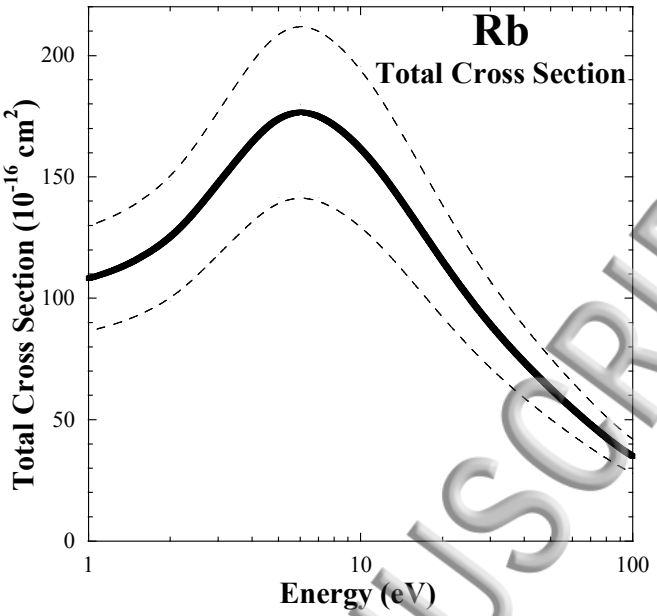

Figure 4.10.1. The recommended total cross section for positron scattering from Rb – solid line. The dashed lines represent the estimated uncertainty limits of ±25% (see also Table 4.10.1).

Table 4.10.2: The positronium formation cross section (in units of 10^{-16} cm^2) for Rb. The estimated uncertainty in these values is ±30% (see also Fig. 4.10.2).

E_0 (eV)	Recommended Positronium Formation Cross Section ($x10^{-16}$ cm^2)
1.0	12
2.0	21
3.0	30
4.0	37
5.0	39
7.5	31
10	22
15	12.5
20	6.5

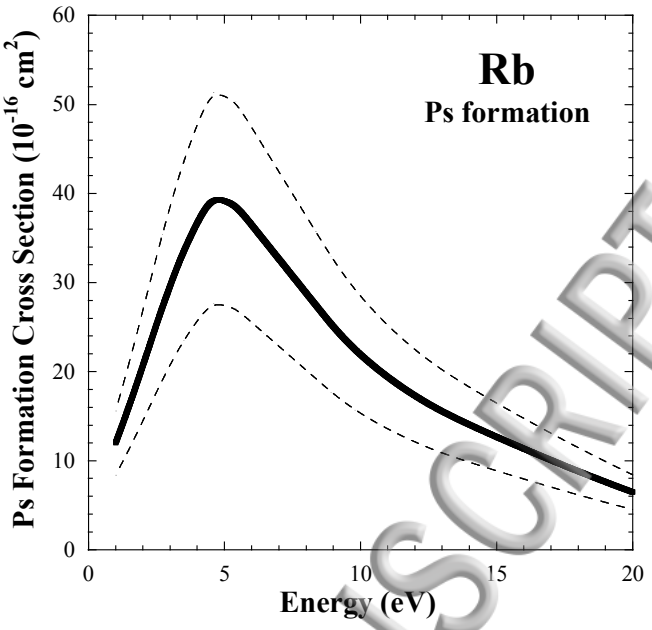

Figure 4.10.2. The recommended positronium formation cross section for Rb - solid line. The dashed lines represent the estimated uncertainty limits of ±30% (see also Table 4.10.2).

4.11 Xenon - Xe

Positron scattering experiments for xenon have yielded measurements of the total scattering cross section [66,162,172,179,252,253,268-270,278], the positronium formation cross section [66,149,182,185,208,209,214,279], and the direct ionization cross section [209,212,213]. There have also been a significant number of theoretical calculations of positron-xenon scattering [97,100,126-129,197,223,227,229,230,255,280-283].

4.11.1 Total Scattering

Total scattering cross section measurements for xenon extend from recent years all the way back to the mid 1970's. As in the other heavier rare gases there appears to be a considerable spread in the absolute values of the measurements, particularly at lower energies where it is apparent that forward scattering effects are most likely responsible for the majority of the differences.

The total scattering data was recently analysed by Chiari and Zecca [11] and they provided a recommended cross section based on their analysis. They comment that their recommended values below 1 eV may be too low due to forward scattering effects which are not completely accounted for in the experiments, and a recent many-body theory calculation [129] indicates this may in fact be the case. While further experiment would be useful to verify this, we suggest that the values of Chiari and Zecca can probably be raised by around 10% for energies below about 1 eV.

Thus our recommended total cross section is identical to that of Chiari and Zecca, with the lower energy values raised by a further ~10%. These recommended values are given in Table 4.11.1 and shown in Figure 4.11.1. The estimated uncertainty on these cross section values is ±10%.

4.11.2 Positronium Formation

There have been a number of absolute measurements of the Ps formation cross section for Xe, dating back to the early 1980's. The level of agreement amongst the various measurements is reasonably good, with the cross section showing a maximum of just under 10 $Å^2$ at an energy of around 10 eV. The comparison between experiment, and between experiment and theory, has been discussed in some detail by Chiari and Zecca in their recent review [11], who also point out, as in the case of argon, that there remains some uncertainty around the existence or otherwise of a second maxima in the Ps cross section near 20 eV. However, Chiari and Zecca did not provide a "recommended" cross section for Ps formation in Xe.

Our recommended positronium formation cross section is given in Table 4.11.2 and shown in Figure 4.11.2. The estimated uncertainty on the cross section values is +15%.

4.11.3 Direct Ionization

There have been two experimental determinations of the direct ionization cross section for Xe – by the UCL and San Diego groups [209,212,213]. The measured cross sections are in reasonably good agreement with each other across the energy range where they overlap and they predict a cross section maximum of around 6 $Å^2$ at about 100 eV. There is also a

reasonably good agreement with theory – particularly the two most recent calculations [97,128].

These cross sections were also analysed by Chiari and Zecaa [11] and Laricchia and colleagues [26], but they did not a suggest a recommended cross section.

The recommended direct ionization cross section is given in Table 4.11.3 and shown in Figure 4.11.3. The estimated uncertainty on these values is ±15%.

Table 4.11.1: The total cross section (in units of 10^{-16} cm^2) for positron scattering from xenon (see text for details). A conservative estimate of the absolute error is ±10% (see also Fig. 4.11.1).

Energy (eV)	Recommended TCS (x10^{-16} cm^2)	Energy (eV)	Recommended TCS (x10^{-16} cm^2)
0.25	85.1	6	16.8
0.3	71.0	7	17.9
0.4	56.2	8	18.8
0.5	49.0	9	19.3
0.6	43.1	10	19.4
0.7	39.0	15	19.2
0.8	35.5	20	18.8
0.9	33.5	30	18.1
1	31.0	40	17.0
1.5	24.0	50	16.0
2	20.4	60	14.9
3	16.8		
4	15.6		
5	15.9		

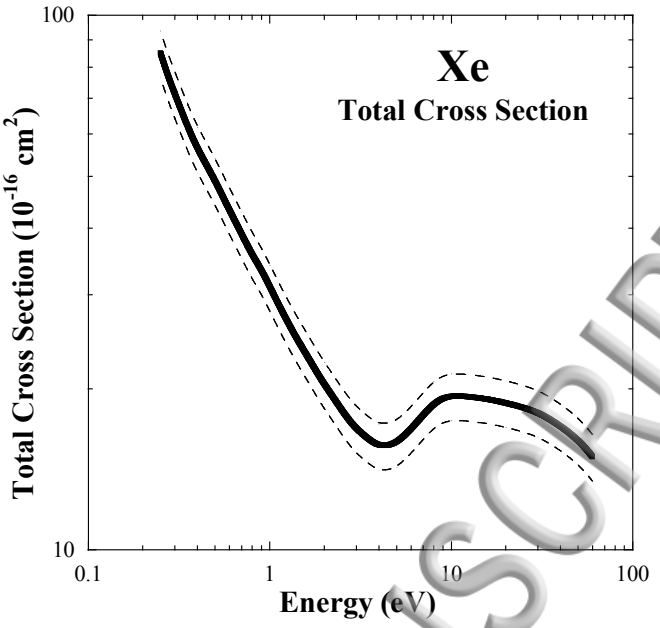

Figure 4.11.1. The recommended total positron scattering cross section for Xe (solid line), while the dashed lines represent the estimated uncertainty limits of ±10% (see also Table 4.11.1).

Table 4.11.2: The positronium formation cross section (in units of 10^{-16} cm^2) for Xe. The estimated uncertainty on these values is ±15% (see also Fig. 4.11.2).

E (eV)	Recommended Positronium Formation Cross Section ($x10^{-16}$ cm^2)	E (eV)	Recommended Positronium Formation Cross Section ($x10^{-16}$ cm^2)
5.3	0	25	6.4
6	3.9	30	5.6
7	6.1	40	4.0
8	7.7	50	2.8
9	8.5	60	1.84
10	9.1	70	1.13
11	9.1	80	0.68
12	8.9	90	0.40
15	8.2	100	0.23
18	7.6		
20	7.2		

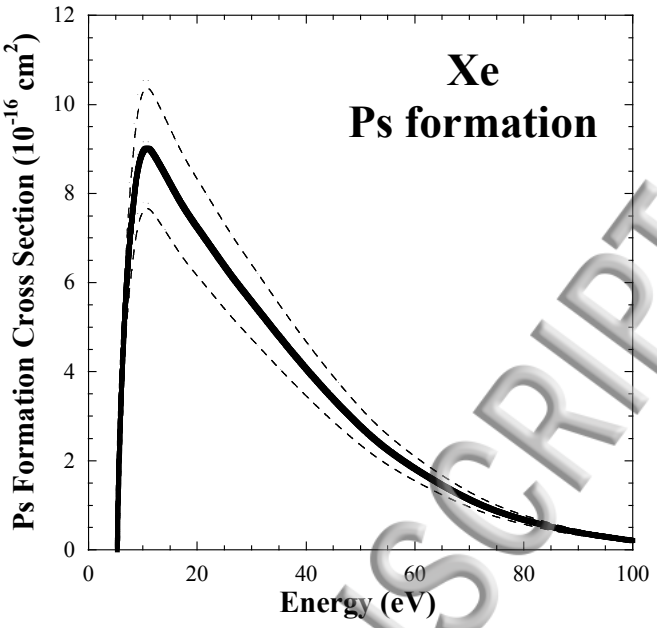

Figure 4.11.2. The recommended total positronium formation cross section for Xe - solid line. The dashed lines represent the estimated uncertainty limits of ±15% (see also Table 4.11.2).

Table 4.11.3: The direct ionization cross section (in units of 10^{-16} cm^2) for positron impact on xenon. The estimated uncertainty on these values is ±15% (see also Fig. 4.11.3).

E_0 (eV)	Recommended Direct Ionization Cross Section ($x10^{-16}$ cm^2)
12.13	0
15	0.60
20	1.68
25	2.91
30	4.20
40	5.82
50	6.26
60	6.34
75	6.26
100	5.97
125	5.46
150	4.97
200	4.08
500	2.13
750	1.52
1000	1.07

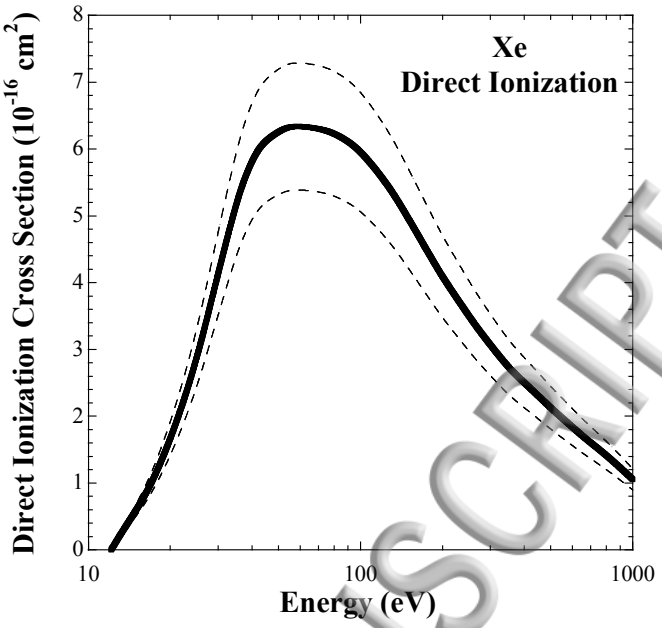

Figure 4.11.3. The recommended direct ionization cross section for positron impact on Xe - solid line. The dashed lines represent the estimated uncertainty limits of ±15% (see also Table 4.11.3).

ACKNOWLEDGEMENTS

We are grateful for the support of the Australian Research Council (Grants DP140102854, DP150101521, DP190100696), and of our respective institutions – The University of Malaya, Flinders University and the Australian National University.

REFERENCES

[1] L. Campbell and M.J. Brunger, Plasma Sources Sci. Technol. **22** 013002 (2013)

[2] B. Boudaiffa, P. Cloutier, D. Hunting, M.A. Huels and L. Sanche Science **287** 1658 (2000)

[3] A. Zecca, L. Chiari, A. Sarkar, S. Chattopadhyay and M.J. Brunger Nucl. Instrum. Meth. B **268** 533 (2010)

[4] M. Kimura, O. Sueoka, A. Hamada and Y. Itikawa, Adv. Chem. Phys. **111** 537 (2000)

[5] R.G. Greaves and C.M. Surko Phys. Plasmas **4** 1528 (1997)

[6] J.P. Sullivan, S.J. Gilbert, J.P. Marler, R.G. Greaves, S.J. Buckman and C.M. Surko Phys. Rev. A **66** 042708 (2002)

[7] S.J. Gilbert, R.G. Greaves and C.M. Surko Phys. Rev. Lett. **82** 5032 (1999)

[8] J.P. Sullivan, J.P. Marler, S.J. Gilbert, S.J. Buckman and C.M. Surko Phys. Rev. Lett. **87** 073201 (2001)

[9] F. Blanco, A.M. Roldan, K. Krupa, R.P. McEachran, R.D White, S. Marjanovic, Z.Lj. Petrovic, M.J. Brunger, J.R. Machacek, S.J. Buckman, J.P. Sullivan, L.Chiari, P. Limao-Vieira and G. Garcia J. Phys. B: At. Mol. Opt. Phys. **49** 145001 (2016)

[10] W. Tattersall, D. Cocks, G. Boyle, M.J. Brunger, S.J. Buckman, G. Garcia, Z.Lj. Petrovic, J.P. Sullivan, and R.D. White Plasma Sources Sci. & Tech. **26** 045010 (2017)

[11] L. Chiari and A. Zecca Eur. Phys. J. D **68** 297 (2014)

[12] T.C. Griffith and G.R. Heyland Phys. Rep. **39** 169 (1978)

[13] T.S. Stein and W.E. Kauppila Adv. At. Mol. Phys. **18** 53 (1982)

[14] W.E. Kauppila and T.S. Stein Adv. At. Mol. Opt. Phys. **26** 1 (1990)

[15] M. Charlton and J.W. Humberston, *Positron Physics* (Cambridge University Press, Cambridge, 2001)

[16] C.M. Surko, G. Gribakin and S.J. Buckman J. Phys. B: At. Mol. Opt. Phys. **38** R57 (2005)

[17] G. Laricchia, S. Armitage, A. Kover and D.J. Murtagh Adv. At. Mol. Opt. Phys. **56** 1 (2007)

[18] J.R. Danielson, D.H.E. Dubin, R.G. Greaves and C.M. Surko Rev. Mod. Phys. **87** 247 (2015)

[19] M.J. Brunger, S.J. Buckman and K. Ratnavelu J. Phys. Chem. Ref. Data **46** 023102 (2017)

[20] J.P. Sullivan, C. Makochekanwa, A. Jones, P. Caradonna, D.S. Slaughter, J. Machacek, R.P. McEachran, D.W. Mueller and S.J. Buckman J. Phys. B: At. Mol. Opt. Phys. **44** 035201 (2011)

[21] O. Sueoka, S. Mori and A. Hamada J. Phys. B: At. Mol. Opt. Phys. **27** 1453 (1994)

[22] P.G. Coleman and J.T. Hutton, Phys. Rev. Lett. **45** 2017 (1980)

[23] J.P. Sullivan, S.J. Gilbert, J.P. Marler, R.G. Greaves, S.J. Buckman and C.M. Surko Phys. Rev. A **66** 042708 (2002)

[24] T.C. Griffith, G.R. Heyland, K.S. Lines and T.R. Twomey J. Phys. B: At. Mol. Phys. **12** L747 (1979)

[25] D. Fromme, G. Kruse, W. Raith and G. Sinapius Phys. Rev. Lett. **57** 3031 (1986)

[26] N.F. Mott and H.S.W Massey *The Theory of Atomic Collisions* (Clarendon Press, Oxford, 1933)

[27] H.S.W. Massey and C.B.O. Mohr Proc. Phys. Soc. A**67** 695 (1954)

[28] J.W. Humberston Adv. Atom. Mol. Phys. **15** 101 (1979)

[29] A.S. Ghosh, N.C. Sil and P. Mandal Phys. Rep. **87** 313 (1982)

[30] A.S. Kadyrov and I. Bray J. Phys. B: At. Mol. Opt. Phys. **49** 222002 (2016)

[31] J. Tennyson, Phys. Rep. **491** 29 (2010)

[32] S.J. Buckman and J.P Sullivan Nucl. Instr. Meth. Phys. Res. B **247** 5 (2006)

[33] E.A.G. Armour Phys. Rep. **169** 1 (1988)

[34] A.S. Ghosh and T. Mukherjee Can. J. Phys. **74** 420 (1996)

[35] R.N. Hewitt, C.J. Noble and B.H. Bransden J. Phys. B: At. Mol. Opt. Phys. **23** 4185 (1990)

[36] K. Higgins and P.G. Burke J. Phys. B: At. Mol. Opt. Phys. **24** L343 (1991)

[37] J. Mitroy Aust. J. Phys. **46** 751 (1993)

[38]M.T. McAlinden, A.A. Kernoghan and H.R.J. Walters Hyp. Int. **89** 161 (1994)

[39] A.S. Kadyrov and I. Bray Phys. Rev. A**66** 012710 (2002)

[40] P.G. Burke, K. Smith and H. Schey Phys. Rev. **129** 1258 (1963)

[41] S.J. Ward, M.Horbatsch, R.P. McEachran and A.D. Stauffer J. Phys. B: At. Mol. Opt. Phys. **22** 1845 (1989)

[42] S.J. Ward, M. Horbatsch, R.P. McEachran and A.D. Stauffer, Nucl. Instr. Meth. Phys. Res. B **42** 472 (1989)

[43] S.J. Ward, M. Horbatsch, R.P. McEachran and A.D. Stauffer J. Phys. B: At. Mol. Opt. Phys. **21** L611 (1988)

[44] R.P. McEachran, M. Horbatsch and A.D. Stauffer J. Phys. B: At. Mol. Opt. Phys. **24** 1107 (1991)

[45] H.R.J. Walters J. Phys. B: At. Mol. Opt. Phys. **21** 1893 (1988)

[46] W.C.Fon, K.A. Berrington, P.B. Burke and A.E. Kingston J. Phys. B: At. Mol. Opt. Phys. **14** 1041 (1981)

[47] R.N. Hewitt, C.J. Noble, and B.H. Bransden J. Phys. B: At. Mol. Opt. Phys. 24, L635 (1991)

[48] R.N. Hewitt, C.J. Noble, and B.H. Bransden J. Phys. B: At. Mol. Opt. Phys. **26** 3661 (1993)

[49] D. Basu, G. Banerji and A.S. Ghosh Phys. Rev. A**13** 1381 (1976)

[50] D. Basu, M. Mukherjee and A.S. Ghosh J. Phys. B: At. Mol. Opt. Phys. **22** 2195 (1989)

[51] S.E.A. Wakid and R.W. Labahn Phys. Rev. A**6** 2039 (1972)

[52] M.A. Abdel-Raouf, J.W. Darewych, R.P. McEachran and A.D. Stauffer Phys. Lett. A **100** 353 (1984)

[53] J. Mitroy J. Phys. B: At. Mol. Opt. Phys. **29** L263 (1996)

[54] J. Mitroy and K. Ratnavelu Aust. J. Phys. **47** 721 (1994)

[55] G. Ryzhikh and J. Mitroy J. Phys. B: At. Mol. Opt. Phys. **30** 5545 (1997)

[56] I. Bray and A.T. Stelbovics Phys. Rev A**46** 6995(1992)

[57] I. Bray and A.T. Stelbovics Phys. Rev A**48** 4787 (1993)

[58] I. Bray and Stelbovics Phys. Rev A**49** R2224 (1994)

[59] A. Kadyrov and Bray J. Phys. B: At. Mol. Opt. Phys **33** L635 (2000)

[60] R. Utamuratov, A.S. Kadyrov, D. V. Fursa and I. Bray J. Phys. B: At. Mol. Opt. Phys. **43** 031001 (2010)

[61] A.V. Lugovskoy, A.S. Kadyrov, I. Bray and A.T. Stelbovics Phys. Rev. A**82** 062708 (2010)

[62] A.V. Lugovskoy, A.S. Kadyrov, I. Bray and A.T. Stelbovics Phys. Rev. A**85** 034701 (2012)

[63] R. Utamuratov, D.V. Fursa, A.S. Kadyrov, A.V. Lugovskoy, J.S. Savage and I. Bray Phys. Rev. A**86** 062702 (2012)

[64] R. Utamuratov, A.S. Kadyrov, D.V. Fursa, M.C. Zammit and I. Bray Phys. Rev. A**92** 032707 (2015)

[65] A.C.L. Jones, C. Makochekanwa, P. Caradonna, D.S. Slaughter, J.R. Machacek, R.P. McEachran, J.P. Sullivan, S.J. Buckman, A.D. Stauffer, I. Bray and D.V. Fursa Phys. Rev. A**83** 032701 (2011)

[66] J.R. Machacek, C. Makochekanwa, A.C.L. Jones, P. Caradonna, D.S. Slaughter, R.P. McEachran, J.P. Sullivan, S.J. Buckman, S. Bellm, B. Lohmann, D.V. Fursa, I. Bray, D.W. Mueller, and A.D. Stauffer, New J. Phys. **13** 125004 (2011)

[67] C. Makochekanwa, J.R. Machacek, A.C.L. Jones, P. Caradonna, D.S. Slaughter, R.P. McEachran, J.P. Sullivan, S.J. Buckman, S. Bellm, B. Lohmann, D.V. Fursa, I. Bray, D.W. Mueller, A.D. Stauffer, M. Hoshino, Phys. Rev A**83** 032721 (2011)

[68] I.E. McCarthy, B.C. Saha and A.T. Stelbovics Phys. Rev. A**23** 145 (1981)

[69] H. Feshbach Ann. Phys. **19** 287 (1962)

[70] I.E. McCarthy and A.T. Stelbovics Phys. Rev. A**28** 2693 (1983)

[71] B.H. Bransden, I.E. McCarthy, A.T. Stelbovics J. Phys. B: At. Mol. Opt. Phys. **18** 823 (1985)

[72] I.E. McCarthy, K.Ratnavelu and Y.Zhou, J. Phys. B: At. Mol. Opt. Phys. **26** 2733 (1993)

[73] I.E. McCarthy and Y. Zhou Phys. Rev. A**49** 4597(1994)

[74] K. Ratnavelu and K.K. Rajagopal, J. Phys. B: At. Mol. Opt. Phys. **32** L381 (1999)

[75] J. Mitroy J Aust. J. Phys. **49** 919 (1996)

[76] A.A. Kernoghan, D.R.J. Robinson, M.T. McAlinden and H.R.J. Walters J. Phys. B: At. Mol. Opt. Phys. **29** 2089 (1996)

[77] K.K. Rajagopal and K. Ratnavelu Phys. Rev. A**62** 022717 (2000)

[78] M.Z. M.Kamali and K. Ratnavelu Phys. Rev. A**65** 014702 (2001)

[79] N. Natchimuthu and K. Ratnavelu Phys. Rev. A**63** 052707 (2001)

[80] K. Ratnavelu and S.Y. Ng, Chin. Phys. Lett. **23** 1753 (2006)

[81] K. Ratnavelu and W.E. Ong Eur. Phys. J. D **64** 269 (2011)

[82] J.H. Chin, K. Ratnavelu and Y. Zhou Eur. Phys. J. D **66** 82 (2012)

[83] Y. Zhou, K. Ratnavelu and I.E. McCarthy Phys. Rev. A**71** 042703 (2005)

[84] G. Nan , Y. Zhou and Y. Ke Phys. Rev. A**72** 012709 (2005)

[85] C. Cheng and Y. Zhou Phys. Rev. A**73** 024701 (2006)

[86] Y. Cheng and Y. Zhou Phys. Rev. A**76** 012704 (2007)

[87] P.G. Burke and W.D. Robb Adv. Atom. Mol. Phys. **2** 143 (1975)

[88] P.G. Burke, C.J. Noble, and P.Scott, Proc. Roy. Soc. Lond. A: Vol. 410. No. 1839. The Royal Society (1987)

[89] P.G. Burke and K.A. Berrington *Atomic and Molecular Processes-An R-matrix Approach* Institute of Physics Bristol (1993)

[90] K. Higgins, P.G. Burke, and H.R. Walters. J. Phys. B: At. Mol. Opt. Phys. **23** 1345 (1990)

[91] K. Higgins and P.G. Burke J. Phys. B: Atom. Mol. Opt. Phys. **26** 4269 (1993)

[92] M.T. McAlinden, A.A. Kernoghan, and H.R.J. Walters. J. Phys. B: Atom. Mol. Opt. Phys. **29** 555 (1996)

[93] M.T. McAlinden, A.A. Kernoghan, and H.R.J. Walters J. Phys. B: Atom. Mol. Opt. Phys. **30** 1543 (1997)

[94] A.A. Kernoghan., M.T. McAlinden, and H.R.J. Walters. J. Phys. B: Atom. Mol. Opt. Phys. **29** 3971 (1996)

[95] C. P. Campbell, A. T. McAlinden, A. A. Kernoghan and H. R. J. Walters. Nucl. Instr. Meth. Phys. Res. B **143** 41(1998)

[96] K. Bartschat, and P. G. Burke J. Phys. B: Atom. Mol. Opt. Phys. **20** 3191 (1987)

[97] K. Bartschat Phys. Rev. A**71** 032718 (2005)

[98] S.R. Chen, R.P. McEachran and A.D. Stauffer J. Phys. B: At. Mol. Opt. Phys. **41** 025201 (2008)

[99] R.P. McEachran and A.D. Stauffer J. Phys. B: At. Mol. Opt. Phys. **42** 075202 (2009)

[100] R.P. McEachran and A.D. Stauffer J. Phys. B: At. Mol. Opt. Phys. **46** 075203 (2013)

[101] K. Bartschat, R.P. McEachran and A.D. Stauffer. J. Phys. B: At. Mol. Opt. Phys. **21** 2789 (1988)

[102] K. Bartschat, R.P. McEachran and A.D. Stauffer. J. Phys. B: At. Mol. Opt. Phys. **23** 2349 (1990)

[103] R.P. McEachran and A.D. Stauffer. J. Phys. B: At. Mol. Opt. Phys. **23** 4605 (1990)

[104] R.P. McEachran and A.D. Stauffer J. Phys. B: At. Mol. Opt. Phys. **36** 3977 (2003)

[105] D.D. Reid and J.M. Wadehra J. Phys. B: At. Mol. Opt. Phys. **29** L127 (1996)

[106] D.D. Reid and J. M. Wadehra J. Phys. B: At. Mol. Opt. Phys. **30** 2318 (1997)

[107] F.A Gianturco and R. Melissa, Phys. Rev. A**54** 357 (1996)

[108] R.P. McEachran, J.P. Sullivan, S.J. Buckman, M.J. Brunger, M.C. Fuss, A. Munoz, F. Blanco, R.D. White, Z.Lj. Petrovic, P. Limao-Vieira and G. Garcia J. Phys. B: At. Mol. Opt. Phys. **45** 045207 (2012)

[109] F. Blanco and G. Garcia Phys. Rev. A**67** 022701 (2003)

[110] D.D. Reid, and J.M. Wadehra. Phys. Rev. A**50** 4859 (1994)

[111] L. Chiari, A. Zecca, F. Blanco, G. Garcia and M.J. Brunger J. Phys. B: At. Mol. Opt. Phys. **47** 175202 (2014)

[112] A.G. Sanz, M.C. Fuss, F. Blanco, Z. Masín, J.D. Gorfinkiel, M.J. Brunger and G. García Phys. Rev. A **88** 062704 (2013)

[113] A.K. Bhatia Atoms **4** 27 (2016)

[114] T.T. Gien J. Phys. B: At. Mol. Opt. Phys. 23 2357 (1990)

[115] T.T. Gien J. Phys. B: At. Mol. Opt. Phys. **26** 3653 (1993)

[116] T.T. Gien Phys. Rev. A**44** 5693 (1991)

[117] T.T. Gien J. Phys. B: At. Mol. Opt. Phys. **22** L129 (1989)

[118] T.T. Gien J. Phys. B: At. Mol. Opt. Phys. **22** L463 (1989)

[119] A.W. Pangantiwar and R. Srivastava J. Phys. B: At. Mol. Opt. Phys. **21** 4007 (1988)

[120] A.W. Pangantiwar and R. Srivastava J. Phys. B: At. Mol. Opt. Phys. **20** 5881 (1987)

[121] S.N. Nahar and J.M. Wadehra Phys. Rev. A**35** 2051 (1987)

[122] S.N. Nahar and J.M. Wadehra Phys. Rev. A**35** 4533 (1987)

[123] A.T. Le, M.W.J. Bromley and C.D. Lin Phys. Rev. A**71** 032713 (2005)

[124] C.N. Liu, A.T. Lee, T. Morishita, B.D. Esry and C.D. Lin Phys. Rev. A**67** 052705 (2003)

[125] G.G. Ryzhikh, J. Mitroy, and K. Varga J. Phys. B: At. Mol. Opt. Phys. **31** 3965 (1998)

[126] R.I. Campeanu, R.P. McEachran, and A.D. Stauffer Can. J. Phys. **79** 1231 (2001)

[127] R.I. Campeanu, R.P. McEachran, and A.D. Stauffer. Can. J. Phys. **77** 769 (2000)

[128] R.I. Campeanu, R.P. McEachran, and A.D. Stauffer. Nucl. Instr. Meth. Phys. B: **192** 146 (2002)

[129] D.G. Green, J.A. Ludlow, and G.F. Gribakin Phys. Rev. A**90** 032712 (2014)

[130] G.F. Gribakin, and W.A. King J. Phys. B: At. Mol. Opt. Phys. **27** 2639 (1994)

[131] L. Hulthén, K. Fysiogr Sällsk. Lund Förhandl. **14** 21 (1944)

[132] W. Kohn Phys. Rev. **74** 1763 (1948)

[133] C. Schwartz Phys. Rev. **124** 1468 (1961)

[134] R.L. Armstead Phys. Rev. **171** 91 (1968)

[135] A.K. Bhatia Phys. Rev. A**75** 032713 (2007)

[136] A.K. Bhatia Phys. Rev. A**77** 052707 (2008)

[137] M. Gailitis Soviet Phys. JETP **20** 107 (1965)

[138] J. Stein and R. Sternlicht Phys. Rev. A**6** 2165 (1972)

[139] J.W. Humberston and J.B.G. Wallace J. Phys. B: At. Mol. Opt. Phys. **5** 1138 (1972)

[140] J.W. Humberston Can. J. Phys. **60** 591 (1982)

[141] J.W. Humberston. J. Phys. B: At. Mol. Opt. Phys. **17** 2353 (1984)

[142] J.W. Humberston, P. van Reeth, M.S.T. Watts and W.E. Meyerhof J. Phys. B: At. Mol. Opt. Phys. **30** 2477 (1997)

[143] S.K. Houston and R.J. Drachman Phys. Rev. A**3** 1335 (1971)

[144] P. Van Reeth, and J.W. Humberston J. Phys. B: At. Mol. Opt. Phys. **32** L103 (1999)

[145] P. Van Reeth, and J.W. Humberston J. Phys. B: At. Mol. Opt. Phys. **30** L95 (1997)

[146] P. Van Reeth, and J.W. Humberston J. Phys. B: At. Mol. Opt. Phys. **32** 3651 (1999)

[147] S. Zhou, W.E. Kauppila, C.K. Kwan and T.S. Stein Phys. Rev. Lett. **72** 1443 (1994)

[148] S. Zhou, H. Li, W.E. Kauppila, C.K. Kwan and T.S. Stein Phys. Rev. A**55** 361 (1997)

[149] T.S. Stein, M. Harte, J. Jiang, W.E. Kauppila, C.K. Kwan, H. Li and S. Zhou Nucl. Instrum. Meth. B**143** 68 (1998)

[150] W. Sperber, D. Becker, K.G. Lynn, W. Raith, A. Schwab, G. Sinapius, G. Spicher and M. Weber Phys. Rev. Lett. **68** 3690 (1992)

[151] M. Weber, A. Hofmann, W. Raith, W. Sperber, F. Jacobsen and K.G. Lynn Hyperfine Interact. **89** 221 (1994)

[152] A. Hofmann, T. Falke, W. Raith, M. Weber, D. Becker and K.G. Lynn J. Phys. B: At. Mol. Opt. Phys. **30** 3297 (1997)

[153] G. Spicher, B. Olsson, W.Raith, G. Sinapius and W. Sperber Phys. Rev. Lett. **64** 1019 (1990)

[154] G.O. Jones, M. Charlton, J. Slevin, G. Laricchia, A. Kover, M.R. Poulsen and S.N. Chormaic J. Phys. B: At. Mol. Opt. Phys. **26** L483 (1993)

[155] J. Mitroy J. Phys. B: At. Mol. Opt. Phys. **28** 645 (1995)

[156] M.B. Shah, D.S. Elliot and H.B. Gilbody J. Phys. B: At. Mol. Opt. Phys. **20** 3501 (1987)

[157] D.G. Costello, D.E. Groce, D.F. Herring and J.W.M. McGowan Can. J. Phys. **50** 23 (1972)

[158] K.F. Canter, P.G. Coleman, T.C. Griffith and G.R. Heyland J. Phys. B: At. Mol. Opt. Phys. **5** L167 (1972)

[159] B. Jaduszliwer, W.M.C. Keever and D.A.L. Paul Can. J. Phys. **50** 1414 (1972)

[160] B. Jaduszliwer and D.A.L. Paul Can. J. Phys. **51** 1565 (1973)

[161] K.F. Canter, P.G. Coleman, T.C. Griffith and G.R. Heyland J. Phys. B: At. Mol. Opt. Phys. **6** L201 (1973)

[162] K.F. Canter, P.G. Coleman, T.C. Griffith and G.R. Heyland Appl. Phys. **3** 249 (1974)

[163] B. Jaduszliwer and D.A.L. Paul Can. J. Phys. **52** 1047 (1974)

[164] B. Jaduszliwer, A. Nakashima and D.A.L. Paul Can. J. Phys. **53** 962 (1975)

[165] P.G. Coleman, T.C. Griffith, G.R. Heyland and T.R. Twomey Appl. Phys. **11** 321 (1976)

[166] J.R. Burciaga, P.G. Coleman, L.M. Diana and J.D. McNutt J. Phys. B: At. Mol. Opt. Phys. **10** L569 (1977)

[167] A.G. Brenton, J. Dutton, F.M. Harris, R.A. Jones and D.M. Lewis J. Phys. B: At. Mol. Opt. Phys. **10** 2699 (1977)

[168] W.G. Wilson J. Phys. B: At. Mol. Opt. Phys. **11** L629 (1978)

[169] T.S. Stein, W.E. Kauppila, V. Pol, J.H. Smart and G. Jesion Phys. Rev. A**17** 1600 (1978)

[170] P.G. Coleman, J.D. McNutt, L.M. Diana and J.R. Burciaga Phys. Rev. A**20** 145 (1979)

[171] T.C. Griffith, G.R. Heyland, K.S. Lines and T.R. Twomey Appl. Phys. **19** 431 (1979)

[172] G. Sinapius, W. Raith and W.G. Wilson J. Phys. B: At. Mol. Opt. Phys. **13** 4079 (1980)

[173] W.E. Kauppila, T.S. Stein, J.H. Smart, M.S. Dababneh, Y.K. Ho, J.P. Downing and V. Pol Phys. Rev. A**24** 725 (1981)

[174] T. Mizogawa, Y. Nakayama, T. Kawaratami and M. Tosaki Phys. Rev. A**31** 2171 (1985)

[175] G.P. Karwasz Eur. Phys. J. D**35** 267 (2005)

[176] J.P. Sullivan C. Makochekanwa, A. Jones, P. Caradonna and S.J. Buckman J. Phys. B: At. Mol. Opt. Phys. **41** 081001 (2008)

[177] P. Caradonna, A. Jones, C. Makochekanwa, D.S. Slaughter, J.P. Sullivan, S.J. Buckman, I. Bray and D.V. Fursa Phys. Rev. A**80** 032710 (2009)

[178] K. Nagumo, Y. Nitta, M. Hoshino, H. Tanaka and Y. Nagashima J. Phys. Soc. Japan **80** 064301 (2011)

[179] S.E. Fayer, A. Loreti, S.L. Andersen, Á. Kövér and G. Laricchia J. Phys. B: At.

Mol. Opt. Phys. **49** 075202 (2016)

[180] T.C. Griffith, G.R. Heyland, K.S. Lines and T.R. Twomey J. Phys. B: At. Mol. Opt. Phys. **12** L747 (1979)

[181] L.S. Fornari, L.M. Diana and P.G. Coleman Phys. Rev. Lett. **51** 2276 (1983)

[182] M. Charlton, G. Clark, T.C. Griffith and G.R. Heyland J. Phys. B: At. Mol. Opt. Phys. **16** L465 (1983)

[183] L.M. Diana, P.G. Coleman, D.L. Brooks, P.K. Pendleton and D.M. Norman Phys. Rev. A**34** 2731 (1986)

[184] N. Overton, R.J. Mills and P.G. Coleman J. Phys. B: At. Mol. Opt. Phys. **26** 3951 (1993)

[185] J. Moxom, G. Laricchia, M. Charlton, A. Kover and W.E. Meyerhof Phys. Rev. A**50** 3129 (1994)

[186] D.J. Murtagh, M. Szluinska, J. Moxom, P. Van Reeth and G. Laricchia J. Phys. B: At. Mol. Opt. Phys. **38** 3857 (2005)

[187] P.G. Coleman, J.T. Hutton, D.R. Cook, and C.A. Chandler Can. J. Phys. **60** 584 (1982)

[188] O. Sueoka J. Phys. Soc. Jpn. **51** 3757 (1982)

[189] S. Mori and O. Sueoka J. Phys. B: At. Mol. Opt. Phys. **27** 4349 (1994)

[190] P. Caradonna, J.P. Sullivan, A. Jones, C. Makochekanwa, D. Slaughter, D.W. Mueller and S.J. Buckman Phys. Rev. A**80** 060701 (2009)

[191] H. Knudsen, L. Brun-Nielsen, M. Charlton and M.R. Poulsen J. Phys. B: At. Mol. Opt. Phys. **23** 3955 (1990)

[192] F.M. Jacobsen, N.P. Frandsen, H. Knudsen, U. Mikkelsen and D.M. Schrader J. Phys. B: At. Mol. Opt. Phys. **28** 4691 (1995)

[193] J. Moxom, P. Ashley and G. Laricchia Can. J. Phys. **74** 367 (1996)

[194] P. Ashley, J. Moxom and G. Laricchia Phys. Rev. Lett. **77** 1250 (1996)

[195] J. Ludlow and G.F. Gribakin Private communication (2004)

[196] H. Wu, I. Bray, D. Fursa and A.T. Stelbovics J. Phys. B**37** L1 (2005)

[197] S. Gilmore, J.E. Blackwood and H.R.J. Walters Nucl. Instrum. Meth. B**221** 129 (2004)

[198] R. Utamuratov, A.S. Kadyrov, D.V. Fursa, I. Bray and A.T. Stelbovics J. Phys. B: At. Mol. Opt. Phys. **43** 125203 (2010)

[199] E. Surdutovich, J.M. Johnson, W.E. Kauppila, C.K. Kwan and T.S. Stein Phys. Rev. A**62** 032713 (2002)

[200] B. Jaduszliwer and D.A.L. Paul Can. J. Phys. **52** 272 (1974)

[201] B. Jaduszliwer and D.A.L. Paul Appl. Phys. **3** 281 (1974)

[202] J.-S. Tsai, L. Lebow and D.A.L. Paul Can. J. Phys. **54** 1741 (1976)

[203] A.G. Brenton, J. Dutton and F.M. Harris J. Phys. B: At. Mol. Opt. Phys. **11** L15 (1978)

[204] M. Charlton, G. Laricchia, T.C. Griffith, G.L. Wright and G.R. Heyland J. Phys. B: At. Mol. Opt. Phys. **17** 4945 (1984)

[205] K. Nagumo, Y. Nitta, M. Hoshino, H. Tanaka and Y. Nagashima Eur. Phys. J. D**66** 81

(2012)

[206] L.M. Diana Proceedings of the 7th International Conference on Positron Annihilation (Eds. P. Jain, R.M. Singru, K.P. Gopinathan World Scientific, Singapore, 1985), p. 428

[207] B. Jin, S. Miyamoto, O. Sueoka and A. Hamada At. Coll. Res. Jpn. **20** 9 (1994)

[208] G. Laricchia, P. Van Reeth, M. Szluinska and J. Moxom J. Phys. B: At. Mol. Opt. Phys. **35** 2525 (2002)

[209] J.P. Marler, J.P. Sullivan and C.M. Surko Phys. Rev. A**71** 022701 (2005)

[210] S. Mori and O. Sueoka At. Coll. Res. Jpn. **10** 8 (1984)

[211] O. Sueoka, B. Jin and A. Hamada Appl. Surf. Sci. **85** 59 (1995)

[212] V. Kara, K. Paludan, J. Moxom, P. Ashley and G. Laricchia J. Phys. B: At. Mol. Opt. Phys. **30** 3933 (1997)

[213] P. Van Reeth, M. Szluinska and G. Laricchia Nucl. Instrum. Meth. B**192** 220 (2002)

[214] M. Szluinska, P. Van Reeth and G. Laricchia Nucl. Instrum. Meth. B**192** 215 (2002)

[215] H. Bluhme, H. Knudsen, J.P. Merrison and K.A. Nielsen J. Phys. B: At. Mol. Opt. Phys. **32** 5237 (1999)

[216] H.S.W. Massey, J. Lawson, D.G. Thompson, in *Quantum Theory of Atoms, Molecules and the Solid State, A Tribute to John C. Slater*, edited by P.-O. Lanowdin (Academic Press, New York, 1966) 203

[217] E.S. Gillespie and D.G. Thompson J. Phys. B: At. Mol. Opt. Phys. **8** 2858 (1975)

[218] E.S. Gillespie and D.G. Thompson J. Phys. B: At. Mol. Opt. Phys. **10** 3543 (1977)

[219] R.I. Campeanu and J. Dubau J. Phys. B: At. Mol. Opt. Phys. **11** L567 (1978)

[220] R.P. McEachran, A.G. Ryman and A.D. Stauffer J. Phys. B: At. Mol. Opt. Phys. **11** 551 (1978)

[221] D.M. Schrader Phys. Rev. A**20** 918 (1979)

[222] H. Nakanishi and D.M. Schrader Phys. Rev. A**34** 1823 (1986)

[223] M.T. McAlinden and H.R.J.Walters Hyperfine Interact. **73** 65 (1992)

[224] K.L. Baluja and A. Jain Phys. Rev. A**46** 1279 (1992)

[225] V.A. Dzuba, V.V. Flambaum, G.F. Gribakin and W.A. King J. Phys. B: At. Mol. Opt. Phys. **29** 3151 (1996)

[226] R.I. Campeanu, R.P. McEachran and A.D. Stauffer Can. J. Phys. **74** 544 (1996)

[227] D.L. Moores Nucl. Instrum. Meth. B**143** 105 (1998)

[228] R.I. Campeanu, R.P. McEachran and A.D. Stauffer Nucl. Instrum. Meth. B**192** 146 (2002)

[229] R.I. Campeanu, L. Nagy and A.D. Stauffer Can. J. Phys. **81** 919 (2003)

[230] L.J.M. Dunlop, G.F. Gribakin Nucl. Instrum. Meth. B**247** 61 (2006)

[231] D. Assafrao, H.R.J. Walters, F. Arretche, A. Dutra and J.R. Mohallem Phys. Rev. A**84** 022713 (2011)

[232] D.V. Fursa and I. Bray New J. Phys. **14** 035002 (2012)

[233] L.A. Poveda, A. Dutra, J.R. Mohallem, Phys. Rev. A 87, 052702 (2013)

[234] C.K. Kwan, W.E. Kauppila, R.A. Lukaszew, S.P. Parikh, T.S. Stein, Y.J. Wan and M.S. Dababneh Phys. Rev. A**44** 1620 (1991)

[235] W.E. Kauppila, C.K. Kwan, T.S. Stein and S. Zhou J. Phys. B: At. Mol. Opt. Phys. **27** L551 (1994)

[236] S. Zhou, S.P. Parikh, W.E. Kauppila, C.K. Kwan, D. Lin, E. Surdutovich and T. S. Stein Phys. Rev. Lett. **73** 236 (1994)

[237] G.G. Ryzhikh and J. Mitroy Phys. Rev. Lett. **79** 4124 (1997)

[238] D.D Reid and J.M. Wadhera Phys. Rev. A**57** 2583 (1998)

[239] A.V. Lugovskoy, R. Utamuratov, A.S. Kadyrov, A.T. Stelbovics and I. Bray Phys. Rev. A**87** 042708 (2013)

[240] T.S. Stein, J. Jiang. W.E. Kauppila, C.K. Kwan, H. Li, A. Surdutovich and S. Zhou Can. J. Phys. **74** 313 (1996)

[241] E. Surdutovich, M. Harte, W.E. Kauppila, C.K. Kwan and T.S. Stein Phys. Rev. A**68** 022709 (2003)

[242] R. Szmytkowski J. de Physique **3** 183 (1993)

[243] G.F. Gribakin and W.A. King, Can. J. Phys. **74** 449 (1996)

[244] R.N. Hewitt, C.J. Noble, B.H. Bransden and C.J. Joachain Can. J. Phys. 74 559 (1996)

[245] R.I. Campeanu, R.P. McEachran, L.A. Parcell and A.D. Stauffer Nucl. Instrum. Meth. B **143** 21 (1998)

[246] H.R.J. Walters private communication cited in [241] above

[247] J. Mitroy and M.W.J. Bromley Phys. Rev. Lett. 98 173001 (2007)

[248] J. Mitroy, J.Y. Zhang, M.W.J. Bromley and S.I. Young Phys. Rev. A**78** 012715 (2008)

[249] J.S. Savage, D.V. Fursa and I. Bray Phys. Rev. A**83** 062709 (2011)

[250] L.A. Poveda, D. Assafrao and J.R. Mohallem Eur. Phys. J. D **70** 152 (2016)

[251] W.E. Kauppila, T.S. Stein and G. Jesion Phys. Rev. Lett. **36** 580 (1976)

[252] P.G. Coleman, J.D. McNutt, L.M. Diana and J.T. Hutton Phys. Rev. A**22** 2290 (1980)

[253] P.G. Coleman, N. Cheesman and E.R. Lowry Phys. Rev. Lett. **102** 173201 (2009)

[254] A. Zecca, L. Chiari, E. Trainotti, D.V. Fursa, I. Bray, A. Sarkar, S. Chattopadhyay, K. Ratnavelu and M.J. Brunger J. Phys. B: At. Mol. Opt. Phys. **45** 015203 (2012)

[255] L.M. Diana, P.G. Coleman, D.L. Brooks, P.K. Pendleton, D.M. Norman, B.E. Seay and S.C. Sharma in Proceedings of the Third International Workshop on Positron (Electron) – Gas Scattering, edited by W.E. Kauppila, T.S. Stein and J.M. Wadehra (World Scientific, Singapore, 1986) 296

[256] T.S. Stein, W.E. Kauppila, C.K. Kwan, S.P. Parik and S. Zhou Hyperfine Interact. **73** 53 (1992)

[257] J.P. Marler, L.D. Barnes, S.J. Gilbert, J.P. Sullivan, J.A. Young and C.M. Surko Nucl. Instrum. Meth. B**221** 84 (2004)

[258] L.D. Barnes, J.P. Marler, J.P. Sullivan and C.M. Surko Phys. Scr. T**110** 280 (2004)

[259] R.E. Montgomery and R.W. LaBahn Can. J. Phys. **48** 1288 (1970)

[260] R.P. McEachran, A.G. Ryman and A.D. Stauffer J. Phys. B: At. Mol. Opt. Phys. **12** 1031 (1979)

[261] S.K. Datta, S.K. Mandal, P. Khan and A.S. Ghosh Phys. Rev. A**32** 633 (1985)

[262] A. Jain Phys. Rev. A**41** 2437 (1990)

[263] S.N. Nahar and J.M. Wadehra Phys. Rev. A**43** 1275 (1991)

[264] L.A. Parcell, R.P. McEachran and A.D. Stauffer Nucl. Instrum. Meth. B**171** 113 (2000)

[265] J. Franz, K. Fedus and G. Karwasz Eur. Phys J. D70 155 (2016)

[266] S.P. Parikh, W.E. Kauppila, C.K. Kwan, R.A. Lukaszew, D. Przybyla, T.S. Stein and S. Zhou Phys. Rev. A **47** 1535 (1993)

[267] M.A. Abdel-Raouf Nuovo Cimento **10** 473 (1988)

[268] M.S. Dababneh, W.E. Kauppila, J.P. Downing, F. Laperriere, V. Pol, J.H. Smart and T.S. Stein Phys. Rev. A**22** 1872 (1980)

[269] M.S. Dababneh, Y.-F. Hsieh, W.E. Kauppila, V. Pol and T.S. Stein Phys. Rev. A**26** 1252 (1982)

[270] P.M. Jay and P.G. Coleman Phys. Rev. A**82** 012701 (2010)

[271] A. Zecca, L. Chiari, E. Trainotti, D.V. Fursa, I. Bray and M.J. Brunger Eur. Phys. J. D **64** 317 (2011)

[272] L.M. Diana, P.G. Coleman, D.L. Brooks and R.L. Chaplin in Atomic Physics with Positrons (Eds. J.W. Humberston, E.A.G. Armour Plenum, New York, 1987) 55

[273] R.P. McEachran, A.D. Stauffer and L.E.M. Campbell J. Phys. B: At. Mol. Opt. Phys. **13** 1281 (1980)

[274] L.T. Sin Fai Lam J. Phys. B: At. Mol. Opt. Phys. **15** 143 (1982)

[275] F.A. Gianturco and D. De Fazio Phys. Rev. A**50** 4819 (1994)

[276] A. Surdutovich, J. Jiang, W.E. Kauppila, C.K. Kwan, T.S. Stein and S. Zhou Phys. Rev. A**53** 2861 (1993)

[277] M.A. Abdel-Raouf Nuovo Cimento D**12** 339 (1990)

[278] A. Zecca, L. Chiari, E. Trainotti and M.J. Brunger J. Phys. B: At. Mol. Opt. Phys. **45** 085203 (2012)

[279] L.M. Diana, D.L. Brooks, P.G. Coleman, R.L. Chaplin and J.P. Howell in Positron Annihilation (Eds L. Dorokins-Vanpraet, M. Dorokins, D. Segers World Scientific, Singapore, 1989) 311

[280] J. Callaway, R.W. LaBahn, R.T. Pu and W.M. Duxler Phys. Rev. **168** 12 (1968)

[281] M. Pai, P. Hewson, E. Vogt and D.M. Schrader Phys. Lett. A**56** 169 (1976)

[282] S.L. Willis, J. Hata, M.R.C. McDowell, C.J. Joachain and F.W. Byron Jr J. Phys. B: At. Mol. Opt. Phys. **14** 2687 (1981)

[283] Z. Chen and A.Z. Msezane Phys. Rev. A **49** 1752 (1994)