Positronium formation in e^+-Li and e^+-Na collisions at low energies

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Measurements of positronium formation cross sections for positrons in the energy range down to a few tenths of one electron volt scattered by Li and Na atoms are reported. The reasonable agreement of the measured cross sections for Li with theoretical predictions is in striking contrast to the case for Na where there is a pronounced divergence between calculated and measured values below 1 eV.

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I. INTRODUCTION

Our group has been measuring total and positronium (Ps) formation cross sections for positrons (e^+'s) scattered by atoms of different alkali metals such as Na, K [1], and Rb [2]. In this paper, we report measurements of Ps formation cross sections (Q_{Ps}) for lithium and measurements for sodium at lower-impact energies.

For all alkali atoms, the Ps formation scattering channel is open at all energies because the binding energy of Ps in the ground state (6.8 eV) is larger than the alkali's ionization energy. This channel plays an especially important role at small energies where e^+ scattering can be very much different from e^- scattering. Early theoretical [using close-coupling approximation (CCA)] calculations [3,4] of total scattering cross sections for K and Rb which did not take the Ps formation channel into account were found to dramatically diverge from the corresponding measurements at low energies, while incorporating this channel in such calculations [5] resolved these discrepancies. Numerous calculations of Q_{Ps} have been performed for different alkali atoms by different groups [5–10], and in many cases, calculations such as those that use the close-coupling approximation that take into account enough states of the target atoms and Ps indicate good agreement with experiments. However, there are still blanks to fill: there have been no experimental results for Q_{Ps} in e^+-Li collisions, and our earlier Na measurements [1] have not been in agreement with the latest sophisticated calculations [6,7]. The lust to fill these blanks has motivated our recent measurements at low-impact energies, and we report their results in this publication.

II. THE SETUP AND PROCEDURE

Although our setup for the measurements has been described in detail in Ref. [1], we provide a brief description below. The positrons originate in a ^{22}Na source, are moderated by a set of tungsten meshes, focused by an electrostatic lens, guided further by an axial magnetic field, then the beam passes through the scattering cell, and it is eventually detected by a channeltron electron multiplier. The scattering cell is a stainless steel oven with a built in heater, thermocouples, and an attached heated cylinder that contains an alkali metal. The metal in the cylinder is melted giving rise to saturated vapor that fills the oven and coats its internal walls. In an ideal situation, the walls are uniformly coated and the saturated vapor pressure (about 0.8 mTorr) is stable and uniform throughout the cell and corresponds to the temperature measured by the thermocouples. As a result, the positron beam is scattered by the vapor of known number density enabling us to measure scattering cross sections.

The positrons gain kinetic energy when they are repelled from the moderator with the applied positive potential with respect to the potential applied to the oven. There is also an energy shift related to the difference in positron affinity to the surfaces of the moderator and the inner oven walls. We use ''retarding curves'' to determine the actual energy of the beam by changing the oven bias voltage with the potential on the moderator fixed. The minimum oven voltage that ''kills'' the beam corresponds to the maximum kinetic energy of the positrons (traveling along the axis). To reduce the energy width of the beam we use a lens-retard element (located in the lens assembly near the ^{22}Na source) that has the applied potential somewhat above the potential at the moderator. This cuts off the slow part of the beam. Then the ideal retarding curve is flat as the oven voltage increases until some point where it rapidly falls off reaching the background value. The actual energy of the beam is determined by the midpoint of the falloff and the energy width by the width of the falloff.

The most obvious consequence of scattering is attenuation of the primary beam. While the total attenuation allows one to measure the total cross section of e^+ scattering by atoms, provided that the angular discrimination is made as good as possible, it is possible to deliberately make the angular discrimination very poor in order to keep the scattered positrons (which have not formed Ps or annihilated otherwise) in the beam with the unscattered positrons; then Ps formation may be the main contribution to the attenuation. Thus, it is possible to measure a so-called ''upper limit'' of Ps formation by measuring the attenuation of the beam, and this has been done as a part of our earlier alkali atom Q_{Ps} measurements [1,2]. This upper-limit signal is comprised of positrons which have formed positronium and positrons which have been scattered into the backward hemisphere or at sufficiently large forward angles that they are effectively removed from the primary beam. However, when the energy of the beam is small, the scattering is not as strongly peaked in the forward direction but rather more uniform, and hence, the effort to keep the elastically scattered positrons in the primary beam may not be as successful at small energies. Indeed, as the energy becomes small (several eV or less), the deviation of

the upper limit from our other Ps measurements increases and approaches the total-cross-section curve. Since the present work has been focused on measurements at low energies, we have chosen not to measure the upper limit.

Positronium formed in the course of the interaction of a positron with an atom is bound to decay: if this is para-Ps (spin 0, relative formation probability 1/4, lifetime 0.125 ns), say with kinetic energy of the order of 1 eV, it travels about 0.5 mm (it does not reach the walls of the scattering cell which are about 3 mm away from the beam) and then decays into two back-to-back gamma rays of 511 keV each; if this is ortho-Ps (spin 1, relative formation probability 3/4, lifetime 142 ns) of the same kinetic energy, it travels about 6 cm. Although ortho-Ps may decay in flight into three gamma rays with the total energy of 1022 keV, it is more likely to hit the walls of the cell (maybe several times) ultimately resulting in two 511 keV gamma rays. Detecting the coincidences of two gamma rays within appropriate energy windows thus allows us to place a lower limit on Q_{Ps} because the two-gamma signal can account for all of the para-Ps and much of the ortho-Ps that is formed in our cell.

The coincident gamma rays are detected by two NaI scintillators attached to photomultiplier tubes located on opposite sides of the scattering cell. The detection efficiency of the two-gamma signal is known [1], and counting the two-gamma coincidences allows us to determine the so-called ''lower limit'' of the Ps-formation cross section. The energy windows of the counting system are set to approximately 511 ± 50 keV and are tuned to catch the 511 keV peak in the detected energy spectrum.

It is also possible to try to detect coincidences of two out of the three gamma rays coming from decays of ortho-Ps by setting the energy windows between 300 and 460 keV. Although, the detection efficiency of this signal is unknown, we did measure this signal and it revealed some interesting features that may open doors to future research.

An axial magnetic field about 90 G in the cell is used to prevent scattered e^+'s from reaching the walls of the cell and producing spurious 511 keV gamma signals. Also, to make the measurements at low energies possible, the magnetization of all stainless steel elements of the apparatus was checked with a gauss meter and the parts with a stray magnetic field above 0.05 G at their surfaces were properly demagnetized. It has also been found that having a fresh coating of the scattering cell's inner walls with the alkali is particularly crucial at small energies of the beam; sometimes getting the beam through the scattering cell is only possible after a preliminary coating. We will further emphasize some other features of measurements at low energies in the analysis of our results.

In this paper, we modified the calculations for Q_{Ps} used in Refs. [1] and [2] where the formula used for the lower limit was

$$Q_{LL} = \frac{Q_T N_{2\gamma} \epsilon_{CEM}}{(N_0 e^{-nQ_T L_a})(1 - e^{-nQ_T D}) \epsilon_{2\gamma} F_\gamma^2}, \qquad (2.1)$$

where Q_T stands for the total e^+-atom cross section, $N_{2\gamma}$ is the rate of two-gamma coincidences, N_0 is the rate of positron counts in the ''cold'' primary beam, n is the alkali atoms number density in the vapor, ϵ_{CEM} is the channeltron efficiency of e^+ detection, $\epsilon_{2\gamma}$ is the two-gamma coincidence detection efficiency, F_γ is the transmission coefficient of gamma rays by the cell's walls, L_a is the beam path length from the entrance aperture of the cell to the front edges of the scintillators, and D is the beam path length between the scintillators. The use of Q_T in this expression assumes that only those positrons in the beam that have not been scattered at all are available for Ps formation. This assumption (although it is not bad when the attenuation is low) is not quite correct, and may be avoided. Since the elastically scattered positrons, or positrons that cause excitation or ionization of the target may still collide with another atom (due to the confining 90 G axial magnetic field) and produce Ps, only the positrons that have formed Ps (para or ortho) are removed from the primary beam and are not available for subsequent Ps formation. Therefore, it is more appropriate to use the above formula with Q_T replaced by Q_{Ps} iteratively, beginning with Q_{Ps} obtained as a limit from Eq. (2.1) as Q_T goes to zero. The following formula provides next iterations for the lower limit:

$$Q_{LL}^{(i+1)} = \frac{Q_{LL}^{(i)} N_{2\gamma} \epsilon_{CEM}}{(N_0 e^{-nQ_{LL}^{(i)} L_a})(1 - e^{-nQ_{LL}^{(i)} D}) \epsilon_{2\gamma} F_\gamma^2}. \qquad (2.2)$$

This iteration procedure does not depend on the total cross section and is free of all uncertainties related with that, and it also converges quite fast: in most cases five iterations are enough. This procedure gives the lower limit and only includes the two-gamma signal. The ''two-out-of-three-gamma'' signal contribution should be calculated using a formula similar to Eq. (2.2) with $N_{2\gamma}$ replaced by the rate of two-out-of-three-gamma coincidences, Q_{LL} replaced by $Q_{2/3\gamma} + Q_{LL}$ (since both the ''two-gamma'' and the ''two-out-of-three-gamma'' signals are the consequences of Ps formation and both of them attenuate the beam), and $\epsilon_{2\gamma}$ replaced by $\epsilon_{2/3\gamma}$, which is a thus far unknown two-out-of-three-gamma detection efficiency. So, if $\epsilon_{2/3\gamma}$ were known, the iterated value of $Q_{2/3\gamma}$ could have been obtained, and then it could have been added to Q_{LL} in Eq. (2.2) to include the attenuation due to the two-out-of-three-gamma signal in the lower limit, and then this process would have been repeated until convergence of the iterations were achieved. In the absence of knowledge of $\epsilon_{2/3\gamma}$, we just assume that for the two-gamma signal, the attenuation of the e^+ beam is only due to this signal alone so it maintains its status of the lower limit. For the two-out-of-three-gamma calculations that are performed assuming the same detection sensitivity as for the two-gamma signal, Q_{LL} is used in the iterations described above, but we do not continue this sequence of iterations because without knowing $\epsilon_{2/3\gamma}$ the further iterations are not sensible.

III. Q_{Ps} IN e^+-Li: RESULTS AND DISCUSSION

Our results for e^+-Li scattering are shown in Fig. 1 and in Table I. In the figure they are compared with the theoretical

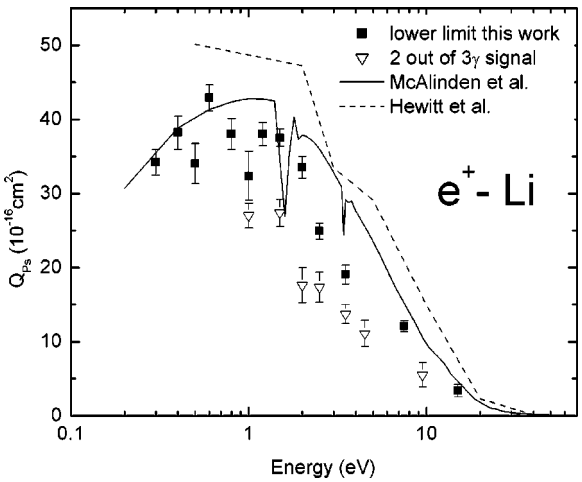

FIG. 1. Ps formation cross-section measurements for e^+-Li scattering along with theoretical calculations by Hewitt *et al.* [5] and McAlinden *et al.* [9]. Statistical uncertainties are represented by error bars except where they are encompassed by the symbols.

coupled-state calculations of McAlinden *et al.* [9] and earlier CCA calculations by Hewitt *et al.* [5]. The agreement with McAlinden *et al.* is reasonable even at the lowest energies: most of the data points are within 15% of the theoretical curve. Our measured values are on the lower side, which makes perfect sense since only two gamma coincidences are taken into account and this, as explained in Sec. II, is a lower limit of Q_{Ps}. If the probability of interaction of ortho-Ps with the cell's walls yielding a two-gamma signal were high, we could argue that the data supports the theory quite well, provided the systematic errors are not too large.

Neither the probability of ortho-Ps conversion at the cell walls nor the two-out-of-three-gamma detection efficiency is known, so we cannot further correct the measured lower limit. The two-out-of-three-gamma contribution for several energy points, also shown in Fig. 1, is calculated assuming the same detection sensitivity as for the two-gamma signal (see Sec. II). The average ratio of this contribution to the lower limit is about 0.7; however preliminary tests suggest that the detection efficiency of the two-out-of-three-gamma signal is larger than that of the two-gamma signal; hence, we expect the actual two-out-of-three-gamma contribution to be smaller than the contribution shown in Fig. 1.

TABLE I. Measured lower limits on Q_{Ps} with statistical errors (shown in parentheses) for e^+-Li scattering.

E (eV)	Q_{Ps} $(10^{-16}$ cm$^2)$
0.3	34.2 (1.7)
0.4	38.2 (2.2)
0.5	34.0 (2.7)
0.6	42.9 (1.7)
0.8	38.0 (2.1)
1.0	32.4 (3.3)
1.2	38.0 (1.6)
1.5	37.5 (1.9)
2.0	33.5 (1.5)
2.5	24.9 (1.1)
3.5	19.1 (1.3)
7.5	12.1 (0.7)
15.0	3.4 (0.8)

The energy width of the beam has not been systematically measured in the Li experiments, but from the Na experiments we know that it is decreasing as the positron energy decreases: $\Delta E \sim 0.75$ eV when $E = 10$ eV, and $\Delta E \sim 0.25$ eV at $E = 0.3$ eV.

IV. Q_{Ps} IN e^+-Na COLLISIONS AT LOW ENERGIES

Earlier positronium formation cross-section measurements in e^+-Na collisions by our group [1] were in agreement with theoretical calculations by Hewitt *et al.* [5]. However, there have been some developments since then: two independent CCA calculations by Campbell *et al.* and Walters *et al.* [7,8], and Ryzhikh and Mitroy [6] suggest that the positronium formation cross sections are expected to level out and even decrease as the energy of the positron beam decreases below 2 eV, which does not agree with our prior measurements. These more recent calculations along with our experience with lithium encouraged us to revisit e^+-Na scattering and make measurements at low energies.

We used the same apparatus as described above and again measured lower limits but not upper limits. We also measured the two-out-of-three-gamma coincidence signal, but we still have not determined its detection sensitivity.

Energy measurements using the retarding curve were taken before and after every cross-section measurement. This allowed us to determine the energy more precisely because it depends on the condition of the coating of the oven's surface with Na. Then the derivative of this dependence with respect to the retarding potential was taken. This derivative is more or less bell shaped, with the maximum corresponding to the average beam energy and the full width at half maximum to the energy width of the beam. Two typical retarding curves along with the derivatives and fits are shown in Fig. 2. One of them is taken at a higher energy, so we can see the flat region and the shape of the energy distribution is very close to a normal distribution. The lens-retard element is used to cut off the beam from the low-energy side narrowing the energy width. The other retarding curve is taken at one of the lowest energies and it does not have the above features. The lens-retard element is not effective at such energies, since there is ''nothing to cut:'' the whole curve is just a tail of the energy distribution resulting from the tungsten moderator. The energy distribution in this tail is not normal. However, there is a steep falloff region at the high-energy side of the distribution, which is due to the cutoff of the longitudinal component of the beam. Therefore, it is most conservative to derive the energy of the beam from that portion of the dependence disregarding the near-zero-energy abnormalities.

The results of our e^+-Na Q_{Ps} measurements are shown in Table II and Fig. 3, where they are compared to the theoretical predictions of Hewitt *et al.* [5], Campbell *et al.* and Walters *et al.* [7,8], and Ryzhikh and Mitroy [6]. It is quite obvious that our results contradict the most recent theories

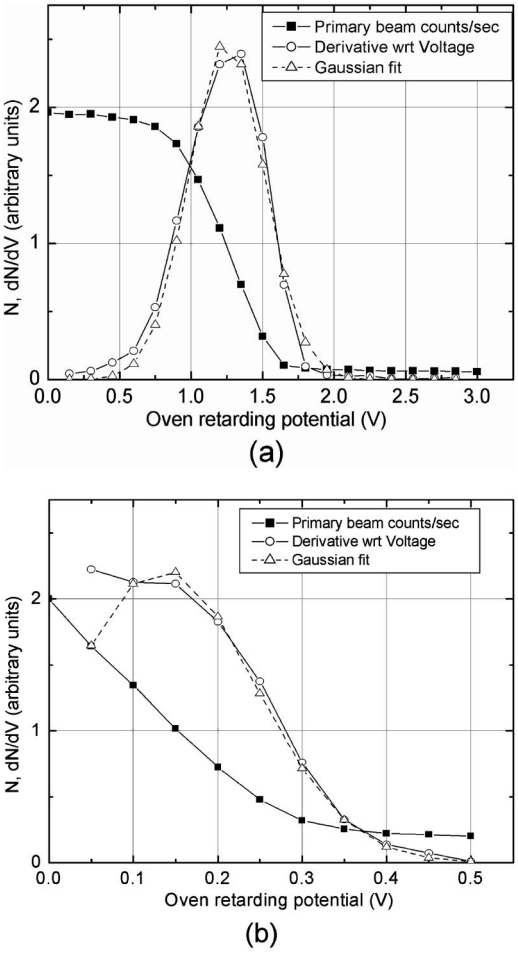

FIG. 2. Typical retarding curves and their derivatives with fitting to determine the energy of the positron beam for energies about 1.25 eV (a) and 0.15 eV (b).

[6–8] at low energies: the experimentally measured Q_{Ps}'s increase rapidly as the energy decreases ($\sim -\log E$) and the theory suggests that Q_{Ps} should rather level out and even decrease. The experimental points depart from the theoretical curve at about 1.25 eV: at 0.2 eV the experimental Q_{Ps} is larger than the theoretical Q_{Ps} by about a factor of 3,

TABLE II. Measured lower limits on Q_{Ps} with statistical errors (shown in parentheses) for e^+-Na scattering.

E (eV)	Q_{Ps} (10^{-16}cm^2)
0.14	83.9 (7.0)
0.22	80.7 (4.8)
0.29	70.1 (6.8)
0.49	64.0 (1.1)
0.70	53.4 (3.0)
1.18	50.0 (3.1)
1.81	39.3 (8.4)
3.25	33.1 (0.9)
5.00	26.4 (1.0)
9.50	13.4 (0.6)

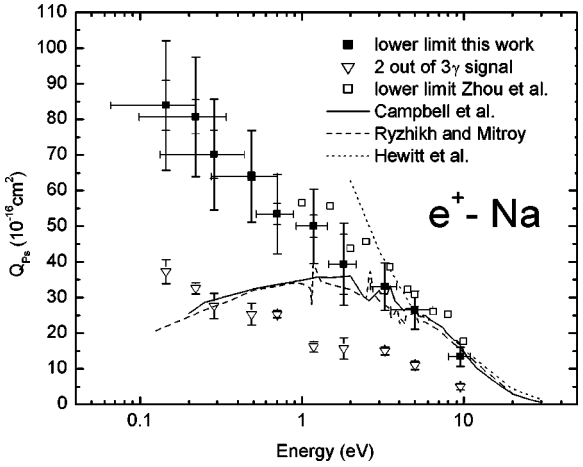

FIG. 3. Ps formation cross-section measurements for e^+-Na scattering along with theoretical calculations by Hewitt *et al.* [5], Ryzhikh and Mitroy [6], and Campbell *et al.* [7]. Statistical uncertainties are represented by the smaller error bars except where they are encompassed by the symbols. Systematic uncertainties (combined in quadrature with statistical uncertainties) for the lower limit are represented by the larger error bars. Error bars are also shown to represent the uncertainty in the positron energies.

while it is within 15% above 2 eV. Because the energy uncertainties at small energies, although smaller compared to those at higher energies, are essentially of the order of the energies, we report the averages of the cross sections whose energies are very close to each other along with the averages of the corresponding energies, weighing them by inverse squares of the statistical uncertainties of the respective measured Q_{Ps}'s and inverse squares of energy widths, respectively.

Our two-out-of-three-gamma measurements, also shown in Fig. 3, have the same trend as the two-gamma lower limit and even if we were to know the corresponding detection efficiency, this would not change the shape of the Q_{Ps} dependence. It is interesting to notice that the ratio of the two-out-of-three-gamma contribution to the two-gamma contribution for Na in Fig. 3 is about 0.5 for all energies while that for Li is approximately 0.7. This might be of special interest in the future if a quantitative analysis allows us to interpret this difference. For now, it suggests that the probability of conversion of the ortho-Ps into a two-gamma signal on the inner walls of the coated scattering cell is higher for Na than for Li.

What could explain the above disagreement between theory and experiment at low energies from an experimental point of view? The statistical errors (shown in Fig. 3), which tend to increase as the energy decreases, are not nearly large enough to cover up the disagreement below 1 eV.

The systematic errors were discussed in detail in Ref. [11]; although that paper was devoted to total-cross-section measurements, a number of the contributions to these errors are similar.

An increase of the measured Q_{Ps}'s at the lowest energies to a greater extent may be due to undercounting of the primary beam as a result of deflections by small stray magnetic and electric fields within the cell. As was mentioned above,

stray magnetic fields were reduced appropriately. The buildup of the alkali on the inner walls of the cell from one measurement to the next slightly modifies the shape of the surface, but fortunately these changes, if substantial, reflect in the tuning of the beam, so we know when we should clean the oven and reload the alkali. All of these tuning parameters were under control and we carefully maintained the same order of procedures in all of our measurements for the Na experiment as well as for the Li experiment.

The lengths L_a and D in formula (2.1) are geometrically measured on the apparatus. Their usage disregards the fact that positrons in the beam move along helixes rather than straight paths, so the effective lengths are longer. Kwan *et al.* [11] estimate that this effect for the total-cross-section measurements is less than 3%. This correction may be slightly larger for the lowest energies, but we are not too apprehensive about this effect also because it is similar for Li and Na measurements and could hardly be the reason for the drastic difference in the shapes of the low-energy e^+-Na Q_{Ps} values.

The errors in determining atom number density for Na are estimated in [11] to be about 21%. This takes into account the uncertainties of saturated vapor pressure dependence taken from Honig and Kramer [12], and the uncertainties in temperature measurements including nonuniformity of the temperature distribution along the cell. The errors for Li are probably somewhat higher because of the higher temperature required.

The energy width may be one of the possible contributions to the above discrepancy. It is expected that the Ps formation cross section becomes infinite at zero energy [7,8]. Because the width of the beam, say, at 0.15 eV is at least 0.15 eV, the beam may contain positrons approaching zero energy and this could account for an increase in the measured Q_{Ps}'s at the lowest energies. We did not go as low in energies with Li, so that could partly explain the lack of disagreement for Li, but the experimental points in Na depart from the theoretical curve around 1 eV, hence the energy width cannot be considered a scapegoat.

In summary, the error analysis does not suggest an explanation for the disagreement between the experiment and theory. The systematic errors combined in quadrature with statistical uncertainties, as well as just the statistical uncertainties by themselves are shown in Fig. 3. Also, it is worth mentioning that the continuous rise of Q_{Ps} at low energies does not appear to be a general feature of the experimental setup, since our Li results as well as our preliminary Mg results do not indicate such an increase at the lowest energies.

There is an indication that the calculations in Refs. [6–9] may be incomplete and they may not accurately describe the lowest-energy e^+ scattering. The predicted bound states of e^+ in both Li and Na by Ryzhikh and Mitroy and Ryzhikh *et al.* [13–15] may change the calculated Q_{Ps} at low energies, but at this point (to the best of our knowledge), the calculations of cross sections including these states have not yet been done. Such calculations may help to explain the difference between Li and Na interactions with positrons.

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