PHYSICAL REVIEW A **76**, 022708 (2007)

Total cross sections for positron scattering from benzene, cyclohexane, and aniline

Antonio Zecca,[1] Norberto Moser,[1] Chiara Perazzolli,[1] Alessandro Salemi,[1] and Michael J. Brunger[2]
[1]*Department of Physics, University of Trento, I-38050 Povo (Trento), Italy*
[2]*ARC Centre for Antimatter-Matter Studies, School of Chemistry, Physics and Earth Sciences, Flinders University, G.P.O. Box 2100, Adelaide, South Australia 5001, Australia*

(Received 4 March 2007; published 15 August 2007)

We use a linear transmission technique to measure total cross sections for positron scattering from benzene, cyclohexane, and aniline. In the case of cyclohexane, the energy range of the present study is 0.1–20 eV, while for benzene and aniline it is 0.2–20 eV. With respect to benzene and cyclohexane, comparison is made to the only other existing results we know of [Makochekanwa and co-workers, Phys. Rev. A **68**, 032707 (2003); **72**, 042705 (2005)]. Agreement with those data is only marginal, being particularly poor at the overlap lower energies. Unlike Kimura *et al.* [J. Phys. B **37**, 1461 (2004)], we find the low-energy dependence of the positron-benzene total cross sections to be qualitatively similar to those found in the electron channel [Gulley *et al.*, J. Phys. B **31**, 2735 (1998)]. We believe that the present positron-aniline total cross sections represent the first time such data have been measured. These cross sections are almost identical to those we found for benzene, suggesting that substitution of hydrogen by the amine group on the aromatic ring is largely irrelevant to the scattering process in the energy regimes considered.

DOI: 10.1103/PhysRevA.76.022708 PACS number(s): 34.85.+x, 25.30.Hm

I. INTRODUCTION

A good review of the available positron–polyatomic-molecule total cross section data, including benzene (C_6H_6) and cyclohexane (C_6H_{12}), is provided by Kimura *et al.* [1]. For completeness we also note the excellent summary of positron–polyatomic-molecule annihilation rates as given by Surko *et al.* [2]. Since the article of Kimura *et al.* [1], relevant studies include those from Makochekanwa *et al.* [3,4], Kimura *et al.* [5], and Sueoka *et al.* [6]. The common link between Refs. [1,3–6] is that all the data contained originate from Sueoka and co-workers. Hence one of the important rationales behind this study is to provide some independent total cross sections against which those from Sueoka and colleagues [1,3,5,6] can be cross-checked. In addition there appear to be no total cross sections for positron-aniline ($C_6H_5NH_2$) scattering, which the present work seeks to rectify. Aromatic amines, for which aniline is a prototypical molecule, are very important in biology and medicinal chemistry. In particular, they play a crucial role in many drugs. Historically, they were also very important in conjugating aromatic rings for applications in the dye industry. From our perspective, we were specifically interested in seeing if replacing hydrogen with an amine group on the aromatic ring would have any effect on the measured total cross sections. Finally, we note that a preliminary study by Karwasz *et al.* [7] touches on some aspects of the present work. However, that preliminary report did not correct for thermal transpiration and *B*-field cyclotron motion effects, nor was the positron beam energy calibrated. The present paper therefore gives the definitive positron-benzene, -cyclohexane, and -aniline total cross sections from Zecca and co-workers.

From a theoretical perspective, none of these scattering systems has been extensively studied. Indeed, to the best of our knowledge, there are in fact no calculations available for either cyclohexane or aniline. For benzene only a continuum multiple scattering (CMS) result from Kimura *et al.* [5] and a "parameter-free" symmetry-adapted, single-center expansion elastic integral cross section from Occhigrossi and Gianturco [8] are available. As the elastic calculation does not include all open channels in the energy regime considered, we would not expect quantitative agreement with the measured total cross section. Nonetheless, as we shall see later, we include it here as we believe its results are instructive.

II. EXPERIMENTAL DETAILS

The positron spectrometer we employed in this study was developed by Zecca and co-workers and has already been described in some previous papers [9,10]. General information about the present attenuation technique can be found, for instance, in Ref. [11]. Although that paper specifically looked at electron cross sections, the two conjugated particles share most of the properties relevant to the present study. Here we therefore outline only those characteristics that are relevant to the present measurements.

Slow positrons (e^+) are produced by a 1 μm tungsten-film moderator in front of a ^{22}Na radioactive source [12]. These positrons are transported and focused into the scattering chamber using a series of charged particle optics with appropriate applied potentials. A 90° electrostatic deflector decouples the scattering and detector region from the source region. Note that a weak axial magnetic field (8–10 G) is also present in the scattering region. The energy resolution of the positron beam has been evaluated to be slightly less than 0.3 eV full width at half maximum, possibly as a result of the partial monochromatization in the deflector and in the optics [9]. In this paper we report cross-section values down to energies of 0.2 eV for benzene and aniline and 0.1 eV for cyclohexane, but values below 0.5 eV are to be regarded as indicative. Indeed, due to the quoted energy spread, the measurements in each gas at energies lower than 0.5 eV (see Tables I–III) should be taken as the convolution of the real (unknown) cross section with the positron energy distribu-

TABLE I. The present total cross section (10^{-16} cm^2) for positron scattering from benzene. The errors represent the standard deviation on the measured cross section at a given energy. See the text for a discussion of the absolute error.

Energy (eV)	Total cross section (10^{-16} cm^2)
0.2	172.7±1.7
0.4	157.5±4.0
0.6	139.6±5.0
0.8	125.0±2.6
1.1	98.7±2.4
1.2	94.8±2.2
1.5	82.7±2.2
1.6	80.0±1.7
1.81	70.8±0.8
2.0	67.0±1.6
2.3	64.3±1.2
2.6	59.7±1.7
2.85	57.1±1.5
3	59.9±1.1
3.1	55.0±1.1
3.3	52.3±0.6
3.4	52.8±0.3
3.6	52.6±0.5
3.8	51.8±0.9
4.1	48.8±0.8
4.6	47.8±0.4
5.6	43.7±0.6
6.6	40.1±1.2
7.6	41.1±1.5
8.6	39.2±0.5
9.6	37.2±1.2
10.6	37.8±0.6
11.6	36.1±0.5
14.6	33.3±0.4
18.1	33.4±0.9

TABLE II. The present total cross section (10^{-16} cm^2) for positron scattering from cyclohexane. The errors represent the standard deviation on the measured cross section at a given energy. See the text for a discussion of the absolute error.

Energy (eV)	Total cross section (10^{-16} cm^2)
0.1	123.9±0.4
0.25	121.6±1.8
0.4	115.8±2.4
0.6	108.0±0.8
1.1	90.0±1.1
1.35	84.2±0.8
1.6	72.0±0.6
2.1	60.4±0.2
2.6	53.4±0.2
3.1	49.5±0.5
3.6	46.5±0.9
4.4	44.1±0.3
5.6	41.8±0.6
6.6	39.7±0.3
7.6	38.4±0.2
8.6	38.0±0.7
9.6	35.3±0.9
10.1	36.9±0.5
10.6	34.3±0.7
11.6	33.9±0.2
12.1	35.7±0.2
13.6	35.5±0.1
14.6	33.5±0.2
18.6	34.2±0.3
19.6	34.1±0.3

tion. Nevertheless, since these are the first measurements at such low energies to our knowledge, it is worth citing them. Using a ^{22}Na source with an activity of 8 mCi, positron beam intensities at the detector were found to vary from about 10 to 130 s^{-1}, depending on the operating conditions, the highest value being achieved at the high-energy limit. The zero for the energy scale of the present positron measurements has been determined, in the absence of the target gases, with a retarding potential analysis of the beam [13]. This measurement suggests a probable error of ±0.1 eV in our energy scale. Our determination of the energy scale calibration is particularly crucial at low energies, where the total cross sections of benzene, cyclohexane, and aniline rise rapidly with decreasing energy. We note that in these instances even a small inaccuracy in the energy calibration can produce a significant uncertainty as to the true value of the total cross section (TCS). Note that such a consideration was not made by Karwasz *et al.* [7] so that their lower-energy data are in significant error. Such an effect would, for example, also be very misleading for theoreticians trying to describe the scattering process in our respective targets of interest. It is known that target gases can affect the true energy zero position by changing the effective emission energy of the projectile particles. We have therefore obtained a check of the insensitivity of our zero-energy determination with the present gases by accurately determining the pass energy in the deflector.

High-purity samples of benzene, cyclohexane, and aniline were used throughout this study and, in addition, each was degassed with freeze-pump-thaw cycles. Each gaseous target was fed to the scattering cell with a two-way diverter valve, where the same amount of gas was diverted to the scattering cell or alternatively was injected into the vacuum system. In the first case attenuation of the positron beam was obtained. With such a provision, we ensure that the background pressure outside the gas cell and therefore the attenuation of the beam in the path outside the gas cell are constant during the measurement cycle. This provision minimizes any effects of the gas on the optical behavior and the quoted influence on the moderator emission properties. The background pressure

TABLE III. The present total cross section (10^{-16} cm^2) for positron scattering from aniline. The errors represent the standard deviation on the measured cross section at a given energy. See the text for a discussion of the absolute error.

Energy (eV)	Total cross section (10^{-16} cm^2)
0.2	167.7±1.8
0.4	162.2±3.3
0.8	128.3±0.7
1.1	99.9±0.6
1.35	100.7±0.3
1.6	84.7±0.7
2.1	66.9±2.3
2.2	67.4±1.0
2.4	66.7±3.1
2.5	58.1±0.5
2.6	61.0±1.3
2.73	57.8±0.3
2.8	58.1±0.9
2.9	59.4±0.7
3.2	58.4±0.6
3.3	55.7±0.4
3.4	53.9±0.1
3.6	54.0±0.9
3.8	50.7±0.7
4.1	49.6±0.3
4.6	47.7±0.3
5.1	49.8±0.6
5.6	43.9±1.6
6.6	42.1±0.7
7.6	41.7±0.5
8.6	40.1±1.5
9.6	39.1±0.6
10.6	38.1±0.1
11.6	38.2±1.9
14.6	34.4±0.9
19.6	32.8±0.5

during the measurements was typically 10^{-3} of the pressure inside the gas chamber.

Total cross sections for each species were computed according to the Beer-Lambert law

$$I_1 = I_0 \exp\left(\frac{-(P_1 - P_0)L\sigma}{kT}\right), \qquad (1)$$

where I_1 is the positron beam count rate at P_1, the pressure measured with the relevant gas routed to the scattering cell, k is Boltzmann's constant, T is the temperature of the gas (K), σ is the total cross section of interest, I_0 is the positron beam count rate at P_0, the pressure with the relevant gas diverted to the vacuum chamber, and L is the length of the scattering region (see later). In order to minimize double-scattering events and ensure that the TCS's are pressure independent for each gas, the ratio I_1/I_0 has been kept to values larger than 0.7. Furthermore, the standard checks on the linearity of the plots of $\ln(I_1/I_0)$ versus gas pressure [14] were performed at selected energies with each species. The geometrical length of the scattering region is 100±0.1 mm, with apertures of 1.5 mm diameter at both the entrance and exit of the scattering chamber. End effects [9] were considered in the present study. It has been demonstrated [15,16] that the effects due to the entrance and exit apertures cancel if the two apertures have equal diameters, so that in our geometry their contribution to the uncertainty in the value of L is possibly less than 0.15%. In the present applications, the value of L used in Eq. (1) has been corrected to account for the path increase caused by the gyration of the positrons in the focusing axial magnetic field (~8–10 G) present in the scattering region (typically this correction is ~6%). The gyration of the projectile particles can also potentially increase the angular resolution error with respect to the no-field case [17]. However, even though absolute differential cross sections for e^+-C_6H_6, e^+-C_6H_{12}, and e^+-$C_6H_5NH_2$ scattering are not currently known [2], so that a correction to our TCS for this effect cannot be made, we believe that the present geometry guarantees a small error (less than 10%) except at the lowest energies—say, below 0.5 eV—where larger errors are possible. The scattering cell pressure has been measured with an MKS Baratron capacitance manometer (Model 628B, 1 Torr full scale) operated at 100 °C. Since the scattering chamber was at room temperature (24±2 °C), a thermal transpiration correction has been applied to the pressure readings. This correction has been calculated according to the model of Takaishi and Sensui [18], and is for each species less than 10% over the entire energy range.

Measurement time was about 1 h per each energy point in each species, with each point being the average of 100 single determinations. The positron beam obtained with our apparatus [10] was extremely stable over times ~1 month, and indeed no influence of any of the target gases on the beam characteristics was noted. The moderator was conditioned at the beginning of our measurements and a new conditioning was not required during the present study. The absolute errors on our measurements (not given in Tables I–III) have been evaluated as the root of the quadratic sum of the contributing errors. A detailed discussion of the origin and of the evaluation techniques of such contributions can be found in Ref. [15] and in the references contained in that paper. The thermal transpiration and B-field corrections have errors bracketed within ±3%; the uncertainty in these corrections can be treated as additional sources of systematic errors but they do not contribute significantly to the overall systematic measurement uncertainty. Overall, the absolute TCS error for each gas typically amounted to ±5% at the higher energies and to ±8% at the lower energies down to about 0.5 eV, the dominant contribution being due to the uncertainty in the pressure determination. At energies lower than this, as noted in the previous paragraph, our cross sections are only indicative, due to the current impossibility of evaluating the angular resolution error: any such error would lead our data to underestimate the true cross section. As a consequence the rate of increase of the TCS at lower energies would be somewhat larger than our data indicate.

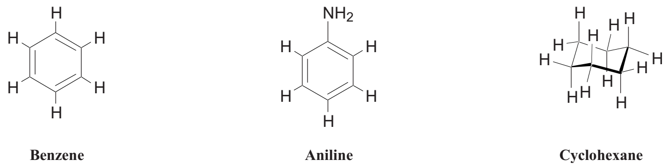

FIG. 1. Schematic representation for the structures of benzene, aniline, and cyclohexane.

III. RESULTS AND DISCUSSION

In this paper we report positron TCS measurements for the molecules benzene, cyclohexane, and aniline, with the structures of these species being schematically represented in Fig. 1. The present total cross section results are plotted in Figs. 2–4, along with previous experimental and theoretical results, where possible, from other groups [3–6,8,19]. Noting the log-log scales of Figs. 2–4, we see that the trends in the energy dependencies of our three TCS's are very similar; namely, they all increase significantly in magnitude as we go to lower energies. Interestingly, the magnitudes of the present TCS's for benzene and aniline are, to within their stated uncertainties, almost identical over the common energy range, while those for cyclohexane are a little smaller. This observation might possibly reflect that, while all three species are cyclic, the structure of cyclohexane is a little different from those of benzene and aniline (see Fig. 1).

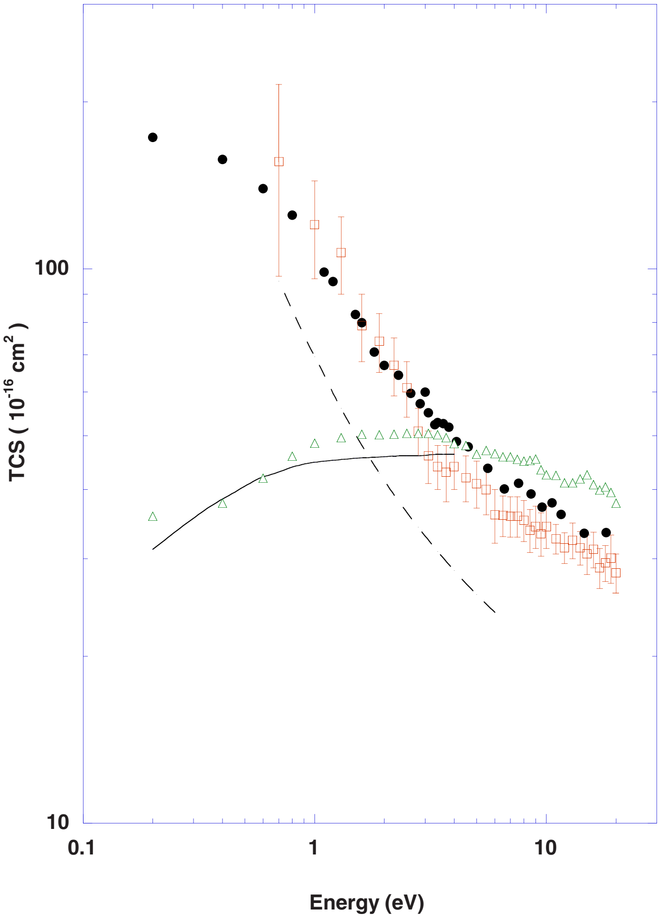

FIG. 2. (Color online) Total cross sections (10^{-16} cm^2) for positron scattering from benzene. The present data (●) are compared with the earlier results from Sueoka (□) [19] and Makochekanwa *et al.* (△) [3]. Also shown are the CMS result (——) from Kimura *et al.* [5] and the elastic ICS calculation (---) from Occhigrossi and Gianturco [8].

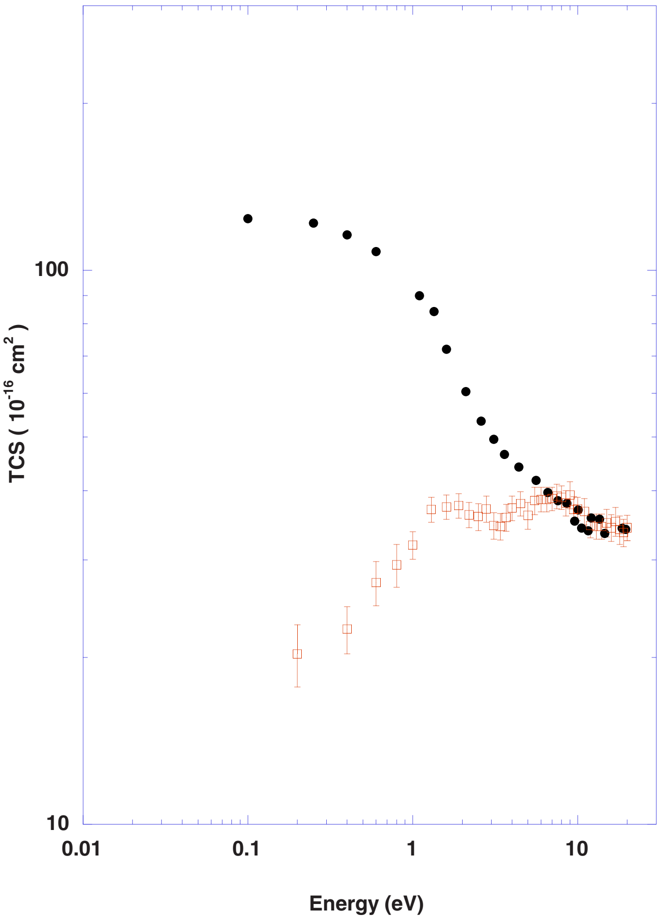

FIG. 3. (Color online) Total cross sections (10^{-16} cm^2) for positron scattering from cyclohexane. The present data (●) are compared with the recent results from Sueoka *et al.* (□) [6].

Considering Fig. 2 in more detail, it is apparent that the present results are in very good agreement with the original benzene TCS measurements of Sueoka [19], across the entire common energy range. Agreement with the more recent measurements from Makochekanwa *et al.* [3] is, however, rather poor. As the apparatus used by Sueoka and co-workers appears to have been pretty much the same for both measurements [3,19], the major difference between their two sets of data appears to be that Sueoka *et al.* (like us) did not correct for forward angle scattering effects, while Makochekanwa *et al.* did attempt to. However, there are no accurate positron-benzene differential cross section (DCS) data available in the literature [2] so that Makochekanwa *et al.* decided to use the elastic electron-benzene DCS results from Cho *et al.* [20]. We do not see *a priori* why using the elastic electron DCS data would be a valid approximation, even to first order. Perhaps more importantly than the above considerations, we stress that any appropriately applied angular resolution cor-

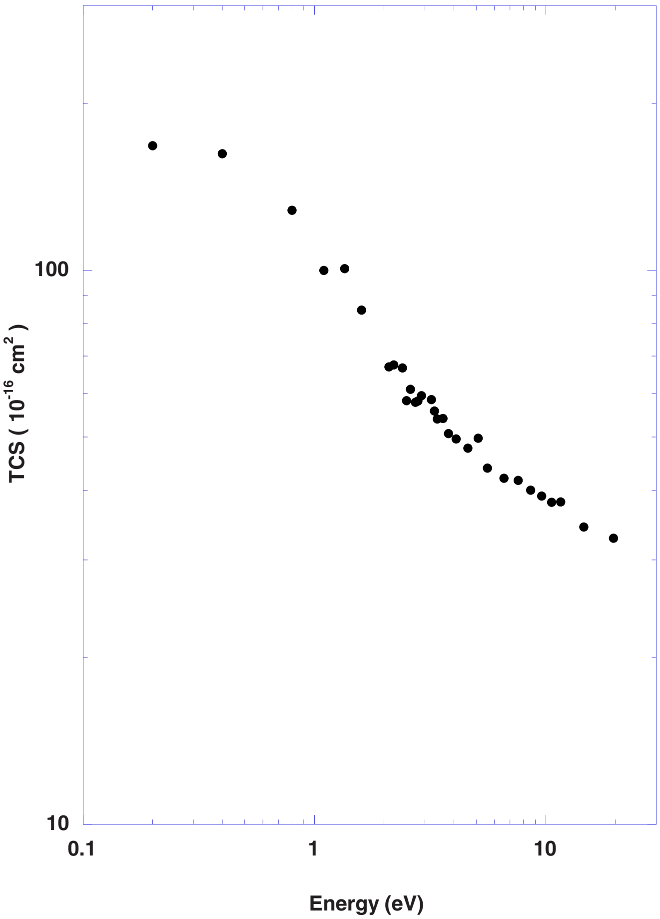

FIG. 4. (Color online) Total cross sections (10^{-16} cm^2) for positron scattering from aniline. The present data (●) are shown.

rection should lead to larger cross-section values. Note also that such corrections, when performed with actual positron differential elastic cross sections, might also have a significant effect on the energy dependence (shape) of the TCS. The former point is verified regarding the positron-cyclohexane measurements of Sueoka *et al.* [6]: they publish both the original and the corrected data, the latter being higher than the former. Therefore it is impossible to ascribe the low TCS values of Makochekanwa *et al.* [3] at energies below a few eV simply to their forward scattering correction. Comparing the two benzene measurements of Sueoka and co-workers, we speculate that the discrepancy below a few eV might be due to an energy-dependent error in [3]. This could be generated by a difference in the measurement procedures they employed in each work [3,19], leading to an energy-dependent improper positron-beam focusing or to an angular resolution distortion in the later study [3]. Further, if we compare the present TCS and that of Sueoka [19] to the elastic integral cross-section (ICS) calculation from Occhigrossi and Gianturco [8] (see Fig. 2) then good qualitative (shape) agreement is found. Note that, as the elastic ICS does not include all open channels, we would not expect quantitative (magnitude) agreement with the TCS. As a consequence, we believe the calculation from Occhigrossi and Gianturco [8] gives more credence to the validity of our data and those from Sueoka [19].

Making a comparison with electron scattering cross sections, we find that the shape of the present benzene TCS is in very good accord with the detailed e^--benzene low-energy TCS results from Gulley *et al.* [21]. This observation is similar to what we have found previously, in comparing low-energy positron and electron TCS's, in H_2O [22] and CO_2 [23], while it is opposite to the conclusion drawn by Kimura *et al.* [5]. Finally, we note that some structure seen (Fig. 2) at around 3 eV in our benzene TCS measurement might be associated with the opening of the positronium channel at around 2.4 eV. Note, however, that the observed energy dependence of this feature is not what one would intuitively expect, around threshold, for the opening of the positronium channel.

A similar type of discrepancy as the above, between the present TCS's and the most recent TCS results from Sueoka *et al.* [6], is also found for positron-cyclohexane scattering (see Fig. 3). As Sueoka *et al.* [6] also attempted to correct their TCS for forward angle scattering effects, by using "synthesized" electron DCS's obtained from normal hexane, it is tempting to ascribe some of the discrepancy observed in Fig. 3 to this. However, as was stressed in the benzene discussion, it is possible that the measurement protocol used in [6] was different from that in Ref. [19], so that there is also an energy-dependent error in the cyclohexane measurements Sueoka *et al.*. Indeed, this could be the main source of the discrepancy between their data and the present. Independent measurements and theoretical calculations are therefore particularly welcome here to try and shed some more light on this scattering system.

Finally, in Fig. 4, we plot the present aniline total cross section measurement. In this case we highlight a small but reproducible structure at around 3 eV. Although we have no explanation, at this time, for its origin, we observe that our cyclohexane TCS shows no such structure in this energy region. Thus we are confident it is not an instrumental effect. Otherwise, to the best of our knowledge, there are no other calculations nor experiments against which we can compare the present results.

IV. CONCLUSIONS

We have reported positron-benzene, positron-cyclohexane and positron-aniline total cross sections for energies in the range 0.1–20 eV. In the case of aniline, we believe this is the first time such data have been reported in the literature, while for benzene and cyclohexane the present results represent the first independent data to be reported. At lower energies, the present benzene and cyclohexane results are generally in rather poor agreement with the most recent measurements from Sueoka's group. We believe we can rule out the possibility that this discrepancy can be ascribed to Sueoka and colleagues using electron DCS's to correct for forward angle scattering effects in their data, although we reiterate this is not physical. A source of this discrepancy might be in the larger uncertainty in the zero-energy determination in Sueoka *et al.*'s apparatus. However, we believe that the major contribution to this discrepancy with their [3,6] most recent data is due to instrumental effects in those measurements. Further theoretical studies into all three of these scattering systems would also be welcome.

ACKNOWLEDGMENTS

This work is supported in part by the Australian Research Council through the Centre for Antimatter-Matter Studies. Financial support from DEST through its International Science Linkages (ISL) scheme is gratefully acknowledged. One of us (M.J.B.) also thanks Flinders University for some Outside Studies Programme (OSP) assistance. European support through the EIPAM Network is also gratefully acknowledged. We all thank L. Campbell for helping us prepare the paper.

[1] M. Kimura, O. Sueoka, A. Hamada, and Y. Itikawa, Adv. Chem. Phys. **111**, 537 (2000).
[2] C. M. Surko, G. F. Gribakin, and S. J. Buckman, J. Phys. B **38**, R57 (2005).
[3] C. Makochekanwa, O. Sueoka, and M. Kimura, Phys. Rev. A **68**, 032707 (2003).
[4] C. Makochekanwa, O. Sueoka, and M. Kimura, J. Chem. Phys. **119**, 12257 (2003).
[5] M. Kimura, C. Makochekanwa, and O. Sueoka, J. Phys. B **37**, 1461 (2004).
[6] O. Sueoka, C. Makochekanwa, H. Tanino, and M. Kimura, Phys. Rev. A **72**, 042705 (2005).
[7] G. P. Karwasz, D. Pliszka, R. S. Brusa, and C. Perazzolli, Acta Phys. Pol. A **107**, 666 (2005).
[8] A. Occhigrossi and F. A. Gianturco, J. Phys. B **36**, 1383 (2003).
[9] A. Zecca, C. Perazzolli, and M. J. Brunger, J. Phys. B **38**, 2079 (2005).
[10] G. P. Karwasz, M. Barozzi, R. S. Brusa, and A. Zecca, Nucl. Instrum. Methods Phys. Res. B **192**, 157 (2002).
[11] B. Bederson and L. J. Kieffer, Rev. Mod. Phys. **43**, 601 (1971).
[12] http://www.tlabs.ac.za/public/default.htm
[13] A. Zecca and M. J. Brunger, in *Nanoscale Interactions and Their Applications: Essays in Honor of Ian McCarthy*, edited by F. Wang and M. J. Brunger (Research Signpost, Trivandrum, India, 2007), p. 21.
[14] R. E. Kennerly and R. A. Bonham, Phys. Rev. A **17**, 1844 (1978).
[15] G. Dalba, P. Fornasini, G. Ranieri, and A. Zecca, J. Phys. B **12**, 3787 (1979).
[16] H. J. Blaauw, F. J. de Heer, R. W. Wagenaar, and D. H. Barends, J. Phys. B **10**, L299 (1977).
[17] A. Hamada and O. Sueoka, J. Phys. B **27**, 5055 (1994).
[18] T. Takaishi and Y. Sensui, Trans. Faraday Soc. **59**, 2503 (1963).
[19] O. Sueoka, J. Phys. B **21**, L631 (1988).
[20] H. Cho, R. J. Gulley, K. Sunohara, M. Kitajima, L. J. Uhlmann, H. Tanaka, and S. J. Buckman, J. Phys. B **34**, 1019 (2001).
[21] R. J. Gulley, S. L. Lunt, and D. Field, J. Phys. B **31**, 2735 (1998).
[22] A. Zecca, D. Sanyal, M. Chakrabarti, and M. J. Brunger, J. Phys. B **39**, 1597 (2006).
[23] A. Zecca, C. Perazzolli, N. Moser, D. Sanyal, M. Chakrabarti, and M. J. Brunger, Phys. Rev. A **74**, 012707 (2006).