

Total cross sections for positron scattering on benzene – angular resolution corrections

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Abstract

We compare recent measurements of total cross sections for positron scattering in benzene from Trento laboratory [G.P. Karwasz, R.S. Brusa, Z. Idziaszek, A. Karbowski, *Eur. J. Phys. D* 144 (2007) 197] with early [O. Sueoka, *J. Phys. B* 21 (1988) L631], later [O. Sueoka, M.K. Kawada, M. Kimura, *Nucl. Instr. Method. Phys. B* 171 (2000) 96] and the most recent [C. Makohekanwa, O. Sueoka, M. Kimura, *Phys. Rev. A* 68 (2003) 32707-1] data from Tokyo laboratory. The latter data are significantly lower than the two other sets. A simple calculation shows that an angular resolution correction, rising strongly in the limit of zero energy, should be applied to measured values if wide apertures in the scattering cell and or strong guiding magnetic fields are used. We show, with the help of the modified effective range theory, that the data from Trento and those of Sueoka (1988) would agree well with those of Sueoka et al. (2000) if the data from Sueoka et al. (2000) were artificially low, as a result of the big angular resolution error due to the experimental conditions present in Sueoka et al. (2000).

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1. Introduction

Although there is a long history of positron scattering experiments, see for example [1,2] and quite sophisticated recent measurements, like the ionization processes [3] or Feshbach vibrational resonances in molecules [4], total cross sections data has only come from a few laboratories. Apart from some pioneering measurements with low intensity positron sources, most extended measurement campaigns were performed at Wayne State University in Detroit covering atomic gases [5] and simple molecules [6], University College London [7] and University of Bielefeld for similar targets [8]. More than 70 molecular targets were, in turn, measured at Tokyo University [9]. Compar-

ing these sets of data, and also recent measurements from Trento laboratory [10] one notices a systematic difference for many targets between the more recent (will discuss this distinction later on) data from Tokyo laboratory and other experiments: Tokyo data tend to fall in the limit of zero energy while other experiments, both on molecules and atoms show rising cross sections. This is, for example, the case for recent data in CO₂, compare [11,12]. Also theories show, for the majority of targets of which we are aware, cross sections rise in the limit of zero energy [13,14]. As these differences in some instances are by a factor of a few folds, we undertook an analysis of possible systematic errors in total cross sections measurements. The most obvious source leading to underestimation of measured total cross sections in the limit of zero energy appears to be the angular resolution error, i.e. counting a fraction of positrons scattered at low angles as non-scattered.

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For the detailed analysis of the angular resolution error in positron scattering we chose the case of benzene for three reasons. First, benzene is a model molecule for the whole class of biologically relevant targets. Second, for benzene precise details of the experiment from the Tokyo laboratory were given in the early work [15], allowing a quantitative and not only qualitative analysis. Third, for benzene several sets of apparently different data, see Fig. 2, were published more recently by the Tokyo group [9,16–18].

2. Angular resolution error in positron experiments

In the transmission method the total cross section (TCS) σ is evaluated from the beam attenuation formula

$$I = I_0 \exp(-pl\sigma/kT) \quad (1)$$

where I and I_0 are the beam currents with and without gas in the scattering cell, respectively, l is the length of the scattering cell, p is the gas pressure, T is the temperature of the gas and k is Boltzmann's constant. Due to practical constraints, (i.e. existence of beam entrance and exit apertures in the scattering cell) the measured TCS is lower than the “real” value. This is because projectile particles scattered into small forward angles, below a certain angle θ_0 , can still reach the detector and are counted as non-scattered. Therefore, the measured TCS is given by the formula

$$\sigma = 2\pi \int_{\theta_0 > 0}^{\pi} \frac{d\sigma}{d\omega} \sin \theta d\theta \quad (2)$$

where $d\sigma/d\omega$ is the differential cross section and θ is the scattering angle (cylindrical symmetry is assumed). Obviously, for the “real” TCS, the angle θ_0 equals to zero.

In electron scattering a common way of comparing the quality of experiments is to give the “angular resolution” defined as the solid angle subtended by the exit aperture from the middle of the scattering cell. For example, the intermediate-energy electron scattering experiment by Możejko et al. [19] is characterised by an order of magnitude poorer angular resolution (3.4×10^{-3} sr) than that of Karwasz et al. [20] (3.1×10^{-4} sr) and almost two orders worse than that of Ariyasinghe et al. [21] (1.2×10^{-5} sr). For electron scattering the angular resolution defined as above is a simple and meaningful feature of experiments. In the limit of high energies and low scattering angles, the differential cross sections are described by the Born approximation and tend to a constant value. Therefore, relative errors due to forward scattering in different experiments are, to the first approximation, proportional to the angular resolution. In the elastic channel they usually amount to a few percent and somewhat more in the inelastic channel, see for example [21] for a detailed discussion. This is not the case in positron scattering – the beams are of low intensities and only sporadically positron experiments can be run on apparatuses dedicated to electron scattering [22]. From the principle of operation of positron apparatuses it turns

out that the angular resolution significantly influences positron TCS and principally in the zero-energy limit.

Up to very recently [4] positron experiments used beams with the intensity varying from a fraction of counts per second [14] to $10^4/s$ [5,6]. Therefore, almost all positron experiments use longitudinal guiding magnetic fields, even if they differ in apparatus details. For example, early experiments from WSU, Detroit were performed inside a long (109 cm) curved solenoid, with entrance and exit apertures of 1.2 and 2.4 mm radii, respectively [5]. Early measurements by Sueoka and Mori [23] in H_2 , N_2 and CO_2 were performed down to 1 eV with a 67.5 mm long scattering cell (we quote the geometrical length and not the “effective” 79.7 mm length) with 4 mm radius apertures and 9 G guiding field. In 1994, Sueoka and Hamada [24] measured again the same targets, with smaller apertures (3 mm in radius) and the magnetic guiding field chosen carefully for each energy range (they used 1.9 G in the energy range up to 2 eV and higher fields at higher energies). In the Trento apparatus a 9 G magnetic field is used with as small as 0.75 mm radius apertures in the scattering cell [25].

Exploring the discrepancies between the different sets of data one notices that the measured value of the TCS decreases significantly (up to factor of a few folds) with larger apertures and greater guiding magnetic field. Therefore, one should not use the geometrical angular resolution to characterize the error in low-energy positron TCS measurements. However, calculating the appropriate angular resolution is trivial, and has already been discussed by Kauppila et al. [5]. It is done by noting the magnetic field causes positrons to spiral around its axis; if the cyclotronic radius is smaller than the exit apertures the positron reaches the detector, independent of the length of the scattering cell.

As this question was not discussed recently and, furthermore, Kimura et al. [18] quoted angular resolution corrections as adopted by Sueoka et al. [27] (i.e. using the concept of the geometrical angular resolution), we give below a sketch essential for defining the appropriate “angular resolution” in positron scattering experiments. The sketch in Fig. 1. illustrates the case of elastic scattering – the projectile velocity v_0 is the same before and after the scattering and the transverse velocity v_{\perp} depends only on v_0 and the

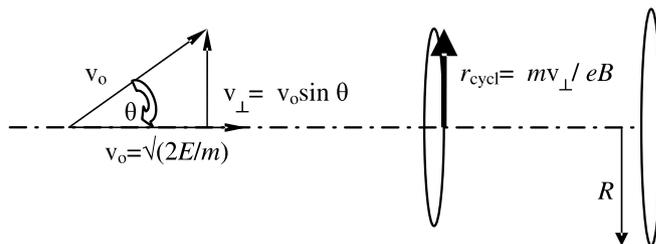


Fig. 1. A schematic drawing for the angular resolution definition in case of positron scattering: scattered positrons with initial energy E are detected as “non-scattered” if their cyclotronic radii r_{cycl} are smaller than the radius R of the exit aperture in the scattering cell.

scattering angle θ . Lowering the projectile energy, for a given scattering angle, the cyclotronic radius lowers. The critical angle θ_0 from Eq. (2), below which all positrons are guided to the detector equals to

$$\theta_0 = \arcsin(eRB/\sqrt{2mE}) \quad (3)$$

where E is the collision energy, B the magnetic field and R the exit aperture radius.

For the sake of comparison, with 9 G field and 4 mm radius R the critical angle amounts to 30° for 4 eV collision energy and 49° for 2 eV; at 1 eV all positrons scattered into angles below 90° are guided to the detector. We can give another synthetic measure of the angular resolution error in positron experiments – we will call it “half value energy”. In the case of a uniform in angle differential cross section this energy corresponds to the critical angle of 90° and the measured TCS would amount to 50% of the real value. The “half value” collision energy equals 0.8 eV in the experiment of Hoffman et al. [6], 1.1 eV in experiment of Sueoka and Mori [23], 0.026 eV in their more recent experiment [24], and as little as 0.0045 eV in Trento experiments [25].

3. Experimental data for benzene

Experimental TCS for benzene, to our knowledge, come only from two laboratories: Trento [26] and Tokyo [14–18]. The Trento apparatus uses a 10 cm long scattering cell with 1.5 mm diameter entrance and exit apertures. The magnetic field is kept between 9 and 9.5 G, with slight adjustments to get optimal beam focusing at given collision energies, see [25] for a detailed description. To summarize possible systematic errors in Trento measurements on benzene we assign 6% value for the possible error in the gas pressure determination (a quadratic sum of the read-out and the thermal transpiration), below 1% for a possible elongation of the electron trajectory inside the scattering cell, 1% to the temperature determination. The statistical error bars (the mean standard deviations of the measured values) are on average 8%.

Tokyo laboratory published TCS for positron and electron scattering from 0.7–400 eV and 1.0–400 eV, respectively [15]. In that paper, details of experimental procedures, in particular the influence of the magnetic field on the measure values, were discussed. With low magnetic field (1.9 G) the TCS rises in the limit of high energy, with an intermediate field (9 G) the TCS is lower in comparisons with the low-field measurements and shows a maximum at 2.5 eV, see Fig. 3, with a high field (23 G) the TCS shows a flat maximum at about 5 eV and falls in the limit of zero energy.

After the pioneering work [15], more sets of data in benzene, visibly different were published by the Tokyo lab: Sueoka et al. [16], Kimura et al. [9], Makochekanwa et al. [17], Kimura et al. [18]. The latter two sets seem to be consistent and show a broad maximum, similar to the

data obtained by Sueoka [15] with a high (23 G) field (compare Figs. 2 and 3). Note also that in the papers by Makochekanwa et al. [17] and Kimura et al. [18] the measured TCS were corrected for the forward scattering by +8% to +12%. This correction was declared to be based on the geometrical angular resolution, similar to that applied by Sueoka et al. in their paper on SiH₄ [27]. Kimura and co-workers [16] used the continuum multiple-scattering method but no details of the potential were given. The results of that theory [16] for electron scattering are lower by about 30% at 2 eV and diverge in the zero-energy limit if compared to other electron experiments [19,28] (which, in fact, rise sharply in the zero-energy limit). We are not aware of experimental details for the data in benzene in [9,16]. The data of Sueoka et al. [16] show a maximum at about 2.5 eV and resemble the early results of Sueoka [15] if obtained with 9 G field (and 4 mm apertures radii), the data reported by Kimura et al. [9] resemble the data by Sueoka [16] but are somewhat higher, see Fig. 2.

In a previous paper we reported data on Ar, H₂, and N₂ [25]. The Trento apparatus yielded cross sections in rather good agreement with data from the Detroit lab [6]. However for N₂, where the comparison was possible, the Trento data were much higher, by almost a factor of three at 1 eV, than those from the Tokyo lab [23,24]. In our paper we performed a possible correction of the data by Sueoka and Mori [23] using their values of the guiding magnetic field (9 G) and scattering cell apertures (4 mm in radius). That calculation was rather easy, as detailed calculations of differential cross sections in nitrogen were given down to 0.001 eV and zero scattering angle [29]. It is not so easy in the case of benzene. We are aware of only one theoretical paper, by Occhigrossi and Gianturco [30]. Their data agree well with the experiment by Sueoka and Mori [31] for C₂H₂, and in benzene the calculation [30] reproduces well the rising TCS in the limit of zero energy but is lower by a factor of two than the experiment from Trento [26] and that of Sueoka [15].

4. Modified effective range theory and “corrected TCS

Due to the lack of published differential cross sections and only a qualitative agreement of the theory by Occhigrossi and Gianturco [30] (and the “computer experiment” character of the theory by Kimura et al. [17]) we adopted our own procedure in order to quantify the angular resolution correction in benzene. Our approach is based on the following procedure. We obtain the scattering potential from integral cross sections and then use this potential to calculate differential data. We analyze the low-energy regime using the modified effective range theory (MERT) with exact solutions of the Schrödinger equation for the long range part of the interaction potential [32]. We perform a MERT fit to the experimental TCS up to 5 eV from the Trento lab [26] and from the early measurement by Sueoka [15] (we use his tabulated data). The MERT procedure allows us to extrapolate the experimental cross section

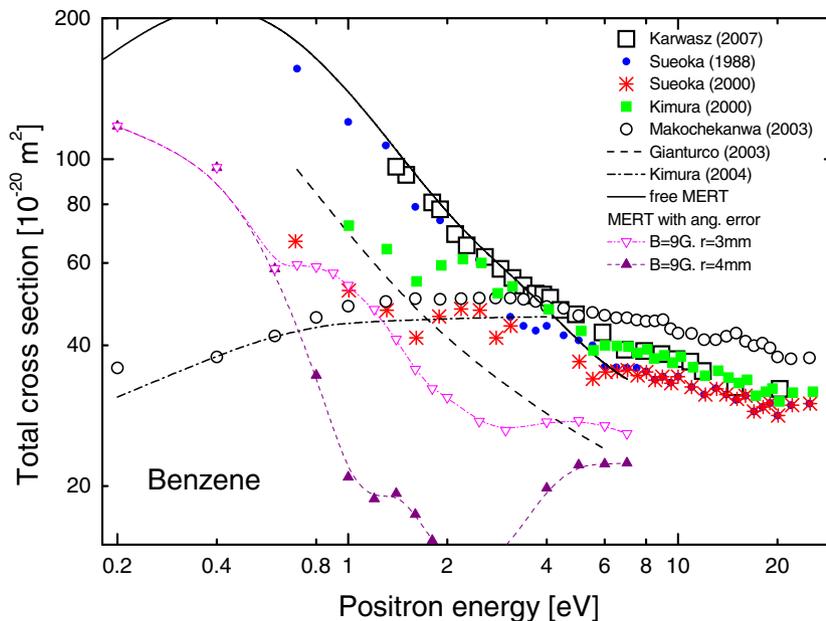


Fig. 2. Total cross sections for positron scattering on benzene. Different set of data from Tokyo lab (circle, [15], tabulated data; stars, [16]; full squares, [9], open circles, [17] and [18]) are compared to the theory by Occhigrossi and Gianturco [30] and CMS (continuum multiple-scattering) method of Kimura [18]. Solid curve is the present unconstrained MERT fit to Trento data (open squares) [26]. Triangles, the MERT fit “corrected” for the angular resolution assuming 9 G guiding field and 3 and 4 mm radius (open and closed triangles, respectively) exit apertures in the scattering cell. Note that tabulated data reported by Sueoka [15] were obtained at 1.9 G field below 2 eV and at higher fields at higher energies (see [15] for the discussion).

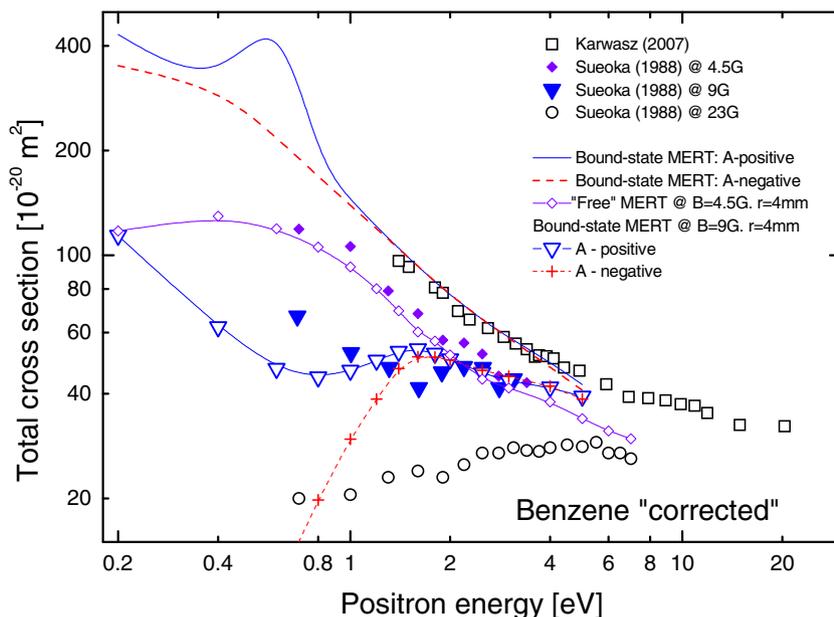


Fig. 3. Total cross sections for positron scattering on benzene. Different sets of data from the early experiment of Sueoka [15] (data obtained digitizing his figures) are compared to data obtained from MERT fit assuming a bound state (with positive or negative scattering length, open triangles and crosses, respectively) and subsequently “corrected” using different experimental angular resolution conditions from [15]. Rhombuses, experimental data of Sueoka [15] obtained with 4 mm radius apertures and 4.5 G magnetic field; triangles, as before but with 9 G field; circles – at 23 G field.

data to the limit of zero energy and to determine the value of the s -wave scattering length.

At large distances the interaction between a positron and a molecule is given by the polarization potential $-\alpha e^2/2r^4$, where α is the dipolar polarizability. The Schrö-

dinger equation for such a potential can be solved exactly (see [32] and reference therein). The solutions are scaled by the characteristic distance $R^* = (\alpha e^2 \mu / \hbar^2)^{1/2}$ and the characteristic energy $E^* = \hbar^2 / 2\mu (R^*)^2$ where μ denotes the reduced mass of the positron-molecule system. The value

of E^* determines the regime where the scattering exhibits low-energy behavior, while R^* is the length-scale of r^{-4} interaction.

In the present MERT analysis we consider the range of energies up to $16E^*$, where there is enough experimental data to perform the fitting procedure. We have applied the semiclassical theory to verify that in this regime of energies the leading contribution comes from s, p and d waves, while the contribution of higher partial waves is small and can be described by taking only the leading order contribution to the phase shift (see [32] for details). In contrast, the phase shifts for $l \leq 2$ are calculated from the exact formulas for the r^{-4} potential [32], where for the short-range parameter $B_l = \tan(\varphi_l + \pi/2)$ we apply the effective range expansion: $B_l(k) = B_l(0) + \frac{1}{2}R_l R^* k^2$. Here k is the relative momentum, φ_l can be interpreted as the short-range phase, and $B_l(0)$ and R_l denote, respectively, the zero-energy contribution and the effective range for the partial wave l . In particular, for $l=0$ the value of $B_l(0)$ is related to the s-wave scattering length through $a = -R^*/B_0(0)$.

Present theoretical MERT fits are compared with the experimental data for benzene in Fig. 2. We have five fitting parameters: a , $B_1(0)$, $B_2(0)$, R_0 and R_1 . We have not included the effective range for d wave, since in the considered range of energies the fitting procedure does not give a reliable value for this parameter. The fitting parameters

and the values of R^* and E^* are presented in Table 1 and differential cross sections at selected energies between 0.2 and 4 eV in Fig. 4.

The obtained differential cross sections were used to produce the set of integral cross sections convoluted with the experimental angular resolution error, using Eq. (1). In Fig. 2 we present two such “corrected” sets, obtained assuming the guiding magnetic field of 9 G and two different apertures in the scattering cell, with 4 and 3 mm radius. As seen from Fig. 2 the “corrected” values are much lower than the TCS from Trento [26] and Sueoka [15]; however, they are not very successful in reproducing the more recent TCS from Tokyo lab either. While the set “corrected” with 3 mm radius agrees pretty well with the data of Sueoka et al. [16] in the 0.5–2 eV energy range, it falls below them at higher energies. The calculation with 9 G and 4 mm radius clearly overestimates the correction needed, see Fig. 2. On the other hand, for the experimental conditions reported by Sueoka [15], 4.5 G and 4 mm apertures, the MERT correction reproduces very well the values measured, see Fig. 3. The question remains, does the differential cross sections produced by an *unconstrained* MERT fit form a unique alternative? Obviously no! The experimental TCSs [15,26] show a somewhat big statistical errors and do not extend to sufficiently low energies. We need to add some constraints to the fit.

Table 1

Five parameters of the present MERT fit to Trento [25] and Sueoka’s [15] TCS performed in the energy range up to 5 eV: a (s-wave scattering length), $B_1(0)$ and $B_2(0)$ (zero-energy contribution for p and d waves), and R_0 , R_1 (effective range for s and p waves in the case of: (1) unconstrained fit and assuming (2) positive and (3) negative scattering length (first to third rows, respectively))

	$R^*(a_0)$	$E^*(\text{eV})$	a/R^*	R_0/R^*	$B_1(0)$	R_1/R^*	$B_2(0)$
Free fit	8.34	0.195	0.30	0.02	0.77	0.20	6.92
$a > 0$	8.34	0.195	1.172	0.101	0.026	0.025	0.106
$a < 0$	8.34	0.195	-1.172	-0.474	0.231	0.235	8.45

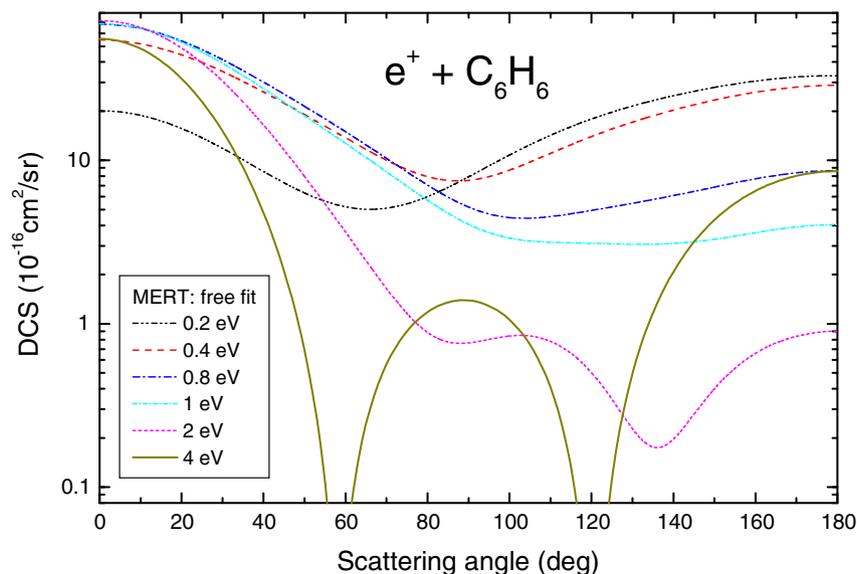


Fig. 4. Differential cross sections for positron-benzene scattering allowing for a free MERT fit to the experimental total cross sections [15,26], see Fig. 2.

During the EMS07 congress Gribakin pointed out to us that benzene shows Feshbach vibrational resonances [4] and following his recent theory [33] should form a virtual bound state at zero energy. Following Gribakin, in this case the integral cross section follows the relation

$$\sigma \propto 1/(k^2 + \kappa^2) \quad (4)$$

with κ^2 being the binding energy and k the scattered positron wave number. Using the experimental results for the binding energy from San Diego lab [4,33] and Trento TCS [26] in the low-energy limit, one obtains an indicative value of the TCS at zero energy of $1200 a_0^2$.

The zero energy constraint still does not suffice to predict the TCS in the energy range which is not covered by experiments. In particular, it is possible that the scattering length a assumes both positive and negative values. (Recall that the zero energy cross sections equals to $4\pi a^2$.) We examined both possibilities and both fits reproduce well the experimentally available TCS past 1 eV. A positive value of a produces a resonance at about 0.5 eV. The differential cross sections obtained by MERT fitting TCS with positive a are shown in Fig. 5.

The two sets obtained with the zero energy constraint were again used for the angular resolution correction. It seems that the MERT fit with positive a performs particularly well. It reproduces not only a maximum in TCS at 2 eV from Sueoka et al. [16] but agrees with those data also at higher energies.

In any case, MERT analysis seems to give a correct indication of how the angular resolution error leads to an underestimation of the TCS by measurements. In order to get more precision, experimental data at lower energies are needed. Then, in spite of the poorer resolution at those energies, the data obtained with high magnetic fields could give a valuable insight into the scattering phenomena.

Namely, by increasing the field with given apertures one tests the contribution of different angular ranges in the TCS value, Eqs. (1) and (2). A necessary requisite is that the experimental conditions (specifically aperture size and magnetic field strength) are carefully recorded.

5. Concluding remarks

In summary, different sets of data from the Tokyo laboratory, apart from the very first measurements by Sueoka [15] with low guiding magnetic field, are lower than the recent data from Trento lab. [26]. The observed discrepancies are qualitatively explained by applying corrections for “angular resolution” (which in the case of positron experiments is totally re-defined from the usual meaning for electron scattering). To obtain reliable corrections both knowledge of exact experimental conditions and theoretical indications on differential cross sections are necessary. We apply the inverted MERT procedure to total cross sections in order to derive the differential cross sections. For small angle corrections, (i.e. in weak fields) the choice of MERT parameters is not critical. However, in order to correct measurements performed with high fields, MERT procedure based on existing data is still ambiguous – measurements at lower energies would be desirable. However, MERT analysis seems to support the suggestion of Gribakin that the benzene total cross section can rise in the limit of low energies, due to presence of a virtual bound state at zero energy. Inverting the reasoning – accurate sets of TCS measurements at different guiding magnetic field (say in the range between a few and few tens of gauss) can indirectly yield differential cross sections and be a stringent test on the theories. Note that such a method (but with the fields in the hundreds of gauss region) lies at the background

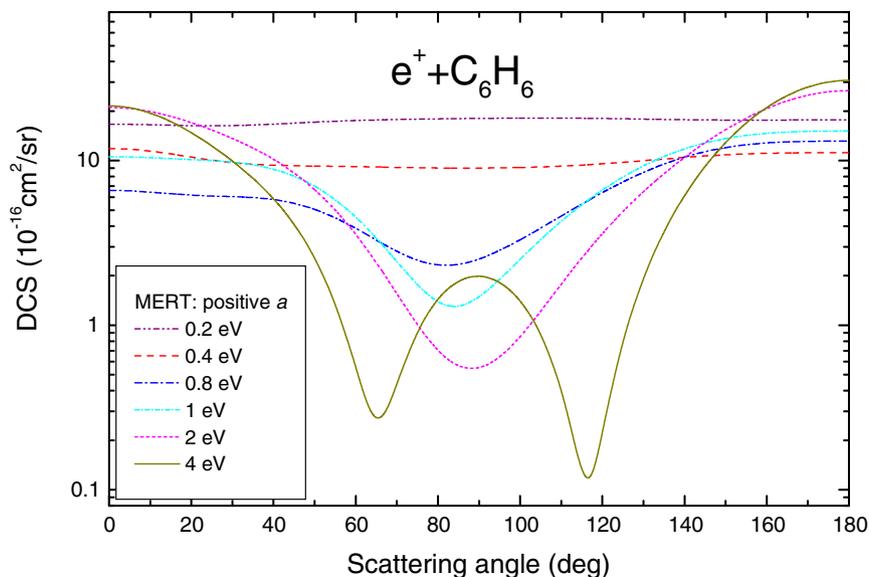


Fig. 5. Differential cross sections for positron-benzene scattering assuming the zero energy TCS equal to $1200 a_0^2$ and using MERT fit to the experimental TCS [15,26], see Fig. 3.

of recent experiments on differential cross sections from San Diego [4] and Canberra [34] laboratories.

Acknowledgements

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