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Energy scale determination and energy resolution in positron total cross section measurements

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Abstract. We compare the recent values of positron total cross sections in benzene, cyclohexane and aniline by Zecca et al. with our previous measurements [Karwasz et al. Acta Phys. Pol. A, 107 (2005) 666] on the same apparatus. An apparent discrepancy disappears if Zecca's data are shifted by +0.2 eV; then their data can be approximated by the modified effective range theory, as well. This observation induced us to compare recent Trento data with other experiments and theories for polar targets, H_2O and HCOOH. The evidence points out towards the need of a careful energy calibration in positron experiments.

1. Introduction

Measurements of total cross sections rarely extend down to sub-eV energy range. This was, for example, the case of the Wayne State University (Detroit) experiment in its early version, using boron ^{11}B radioisotope what allowed to perform measurements of total cross sections in Ar [1] down to as little 0.4 eV while the measurements with a thick (ribbon) W moderator stopped at 4 eV [2]. Recently a new version of the tungsten moderator a thin 1 μm micro foil has been developed at Trento University [3-6], allowing measurements of total cross section down to a few tenths of eV.

Two distinct groups performed measurements on the Trento apparatus [5] – present authors [7-10], and more recently Zecca and collaborators who published data on simple targets as H_2O [11] and on more complex, organic molecules [12-14]. The two sets from Trento apparatus for targets like benzene and aniline apparently differ. The newest-type moderator i.e. the solid Ne, followed by a gas-cell re-moderation stage can yield as good as 25 meV energy resolution [15]. It is currently used at Australian National University in Canberra with the energy resolution of 65 meV [16] and some preliminary data were shown at the present Workshop.

The aim of the present paper is to show some data coming from those recent experiments and compare them with the most recent theories [17]. In particular we discuss the energy scale as used in Zecca's *et al*. reports [11-14]. We show that for all the discussed targets - atoms (He, Ar), hydrocarbons (C_6H_6, C_6H_{12}, C_6H_5N) and polar molecules (H_2O, HCOOH) there exist a very good agreement between the recent theories and (both) sets of Trento experimental results, once a proper energy scale is given. In detail, the analysis shows that the energy calibration in Zecca's data has to be adjusted by some +0.2 eV.

2. Energy scaling procedures

Measurements of electron (and positron) scattering are subject to the energy-bias uncertainty mainly due to electrochemical contact potentials between the source and the scattering cell. The most objective way of determining the energy scale shift are direct measurements of some sharp structures in cross sections, like the resonant vibrational structure in N_2 [18] or sharp resonances in He [19] or Ar [20]. For positrons any sharp structures in cross sections are still a subject of search [21]. In their absence some substituting measures have to be found. The use of electron cross sections, like the N_2 resonant vibrational structure, is one of them. As seen from figure 1, the Trento apparatus with the electron optics set for positron measurements is able to reproduce that structure, and the deduced energy resolution is about 150 meV.

Unfortunately, the methods mentioned above can not be used to determine the energy scale. The work function of positron re-emitted from the tungsten surface is positive while for electrons it is negative. In our apparatus neither the time-of-flight calibration method [15, 22] can be used. Therefore, we have calibrated the energy scale against sharp features like the positronium-formation thresholds in N_2 and Ar [8] which are known with a high accuracy. In particular, in Ar no (rotational, vibrational or electronic) excitations are possible below the Ps threshold (8.96 eV) so the onset is well visible, see figure 2. Furthermore, as seen in our data for Ar, as noted by Szłuińska and Laricchia for Xe [23] and as recently confirmed by Buckman and collaborators in Ar [24], threshold structures are present near the positronium threshold. From Ar measurements we deduced the potential bias of +2.4 eV between the W moderator and the scattering cell. Such a value is in a perfect agreement with measurements of the energy spectrum for positrons emitted from the same-type moderator [25].

The spectrum of positrons emitted from W-moderator is significantly different from that for secondary electrons which extends from zero up to some tens of eV. The Trento apparatus is not equipped with an energy-selector in sensu stricte, see details in figure 1 of Ref. [8]. Three elements perform, however, the energy selecting function: 1) the positron source, yielding a few-eV wide spectrum, 2) the deflection bent, with 1.2 eV FWHM pass-band and 3) the longitudinal magnetic field in the scattering cell. In particular, that latter, as proved in constructing a similar drift-tube [26] for the positron microscope [3], assures the transmission only for positrons at strictly quantified energies (say 2, 4, 6 eV etc.). These three elements perform de facto the monochromatic action on positron, but not on the secondary electrons. For electrons, in particular at low energies, more than one quantified energy can be transmitted through the scattering cell. In fact, as seen from the comparison of Zecca's *et al.* data in tetrohydrofuran [11] with other laboratories [27, 28], his electron data are in a serious error; as a consequence, Zecca has shown no electron data for successive targets.

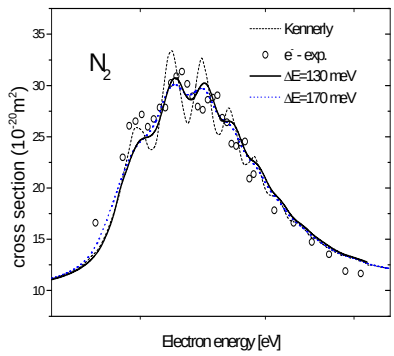

Figure 1. Performance tests (energy resolution evaluation) of Trento [8] apparatus - vibrational resonant structure in N_2 electron-scattering [18] compared to the structure measured with Trento positron-scattering apparatus [8]. The measured structure indicates 130-150 meV energy resolution.

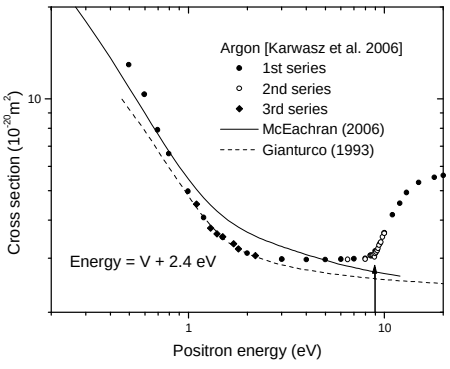

Figure 2. Performance tests (energy calibration) of Trento [8] apparatus for argon. Points – Karwasz et al. [8], separate experimental series. Theory: broken line, Gianturco et al. [29]; solid line, McEachran and Stauffer [30]. The arrow shows the positronium - formation threshold.

3. Comparison of experimental and theoretical data

Comparison of different sets of experimental (and theoretical) data is a supplementary way of determining the construction features of the apparati. For argon we compare our experimental data [8] with two recent theories - by Gianturco *et al.* [29] polarisation potential from free-electron-gas derivation with dipole potential and by McEachran [30] using the complex ab-initio optical potential. The two theories agree pretty well with the experiment and the modified effective-range fit [31]. However, only the theory by Gribakin and Ludlow [32] using many-body theory with perturbation corrections to the correlation potential is able to reproduce the constant value of the cross section between about 2 eV and the positronium-formation threshold. Some spread between theories still does not allow to make decisive judgments and more measurements are needed.

In figure 3 we compare present experiment for benzene with those by Zecca *et al.* [14] and the early data by Sueoka *et al.* [21]; we do not show comparison with some more recent experiments from Tokyo lab, as they were, probably, subject to a big angular-resolution error [33]. Data of Zecca *et al.* almost coincide with ours, but they must be shifted by +0.2 eV. After this shifting, all three sets agree very well up to the positronium-formation threshold (signed by the arrow in fig. 3). Above the positronium-formation threshold the data of Sueoka [22] deviate downwards. This can be explained by opening of this new channel: for rather large (3 mm radius) exit apertures of the scattering cell, the electrically neutral positronium, if formed in the forward direction, can reach the detector and lower the measured cross section. This effect can be superimposed on the confining action of rising values of the magnetic field used at higher energies by Sueoka. Zecca's *et al.* [14] presently corrected values are approximated well also by the modified effective range theory [34].

Also for cyclohexane and aniline, see figure 4, the data by Zecca *et al.* [14], after the energy correction by +0.2 eV, coincide with our results [7]. Present data in cyclohexane (together with corrected results by Zecca [14]) can be well approximated by the MERT fit [33]. The data of Sueoka *et al.* [34] agree with the two Trento sets above 5-6 eV but deviate downwards at lower energies; the angular resolution [34] can be again the reason for the discrepancy. In aniline, only the two Trento sets can be compared: they coincide if the energy scale correction by 0.2 eV is allowed. A bump in the total cross section just above the positronium- formation threshold (signed by an arrow in figure 4) is seen in aniline.

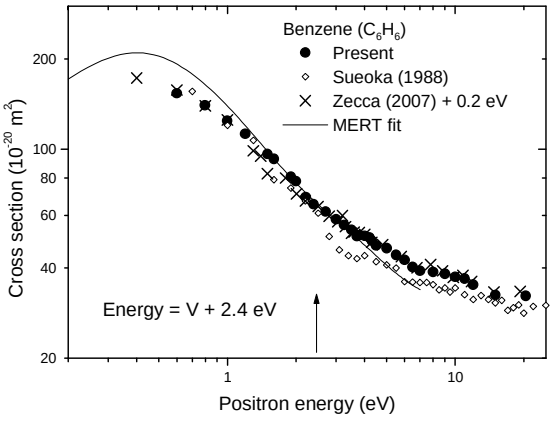

Figure 3. Benzene total cross sections - two sets from Trento are compared – Karwasz *et al.* [7] and Zecca *et al.* [14], the latter shifted by +0.2 eV. The two set coincide with the statistical error bars. The data of Suoeka [22] also coincide, up to 2.7 eV, above where a higher magnetic field was used (9 G instead of 4.5 G). MERT fit from Ref. [33].

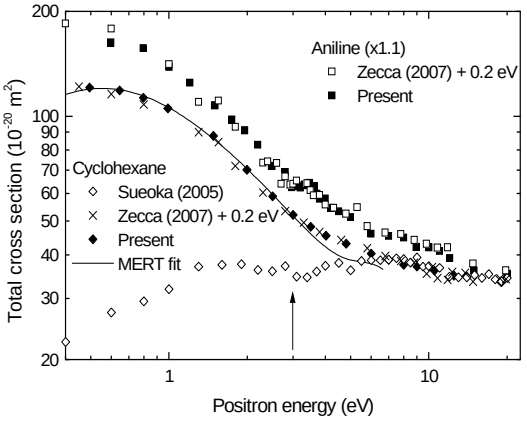

Figure 4. Cyclohexane and aniline cross sections - two experiments from Trento, Karwasz *et al.* [7], and Zecca *et al.* [14] shifted by +0.2 eV. The two set coincide with the statistical error bars. The data of Sueoka *et al.* [34] in cyclohexane are lower that the two Trento sets at low energies, probably due to poorer angular resolution. The aniline data, for clarity, were multiplied by 1.1 factor.

In benzene, Sueoka [22] measured a significant contribution to the total cross section coming from the positronium formation (about 10%) at about the same energies. If a similar contribution was the case of aniline, the bump in the total cross sections would account for the positronium formation process.

In figure 5 we come back to our reporting on resonant structures in He at 1.7 and 2.4 eV [9]. Zecca collaborated at this discovery but successively dissociated, with arguments based exclusively on post-experiment speculations, as we showed in [10]. The most recent experiment from ANU [16], performed with 530 G magnetic field has not confirmed our findings. However, it yielded some single experimental points above the average level at 2 eV and 8 eV. More experiments are needed.

A surprise comes from comparison of our helium data with the most recent, convergent close-coupling, two-centre expansion by Utamuratov *et al.* [35]. Our data agree perfectly with them, both in amplitude and the energy position, but only up to the position of resonances. The theory starts to rise visibly at 2 eV. We recall our original hypothesis [36] that the observed structures mark the opening of a new (i.e. the virtual positronium- formation) scattering channel.

Finally, let us analyze results from Trento on polar molecules, like H_2O [11] and HCOOH [13]. These molecules show a sharp rise in the cross sections in the zero-energy limit, due to their polar character. The recent theory for HCOOH by Bettega and Lima [13] give cross sections significantly higher than those reported from the experiment by Zecca *et al.* [13]. The difference is a high as 30% at 0.5 eV, see figure 3 in [13]. Several possible reasons for the discrepancy were discussed in that paper [13] but not the experimental energy-scale shift. In figure 6 we compare the Bettega and Lima's theory [13] with Zecca's experimental values [13] shifted by +0.3 eV: the two sets agree quite well.

In water the picture is particularly complicated [17]. To our knowledge, for positrons only two theories, single-centre expansion by Gianturco *et al.* [37] and Baluja *et al.* [38] in R-matrix calculations exist in the low energy range. The two theories almost coincide. More theoretical results are available for electron scattering [39, 40], but rather in disagreement, see [41]. However, recently a new experimental result [42] has been obtained for electron scattering using an absolute method and a very precise energy calibration (electrons emitted from photoionization of Ar). Zhang *et al.* [17] have calculated the integral elastic cross sections in R-matrix approximation; their results coincide with the experiment [42]. In the zero energy limit electron (and positron) scattering is dominated by the dipole interaction, so two projectiles should yield similar cross sections. Therefore, in figure 6, apart from experimental data of Zecca *et al.* [11] shifted again by +0.3 eV, we show the rotationally elastic cross sections by Zhang *et a*l.: the two sets almost coincide. Resuming, the measurements on the Trento apparatus performed by Zecca can be validated, but only if the energy scale is carefully re-defined.

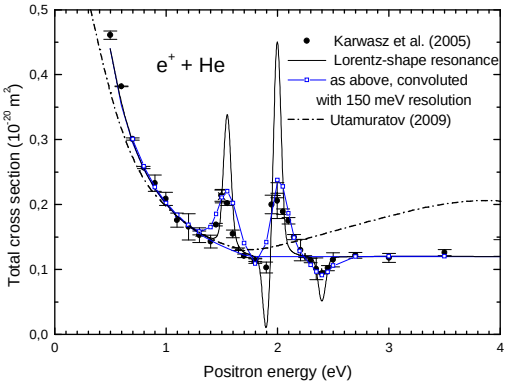

Figure 5. The virtual positronium resonance in He [9, 10, 36] compared to convergent close-coupling theory of Utamuratov *et al.* [35]. The thin lines correspond to a rigid-sphere resonance profile [36], but with the inverted resonant phase-shift ("sticky ball") and 150 meV energy resolution convolution.

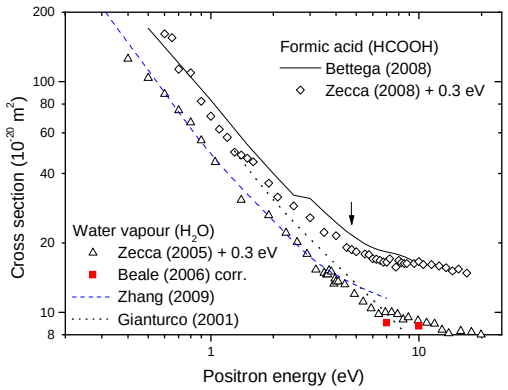

Figure 6. Positron-scattering cross sections: Zecca *et al.* for H_2O [11] and HCOOH [13], corrected by +0.3 eV; Beale *et al.* [44] as corrected by Zhang *et al.* [17]. Theory: HCOOH, Bettega and Lima [13]; H_2O, Gianturco et al. [37], Zhang *et al.* [17] electron scattering, in agreement with [42].

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References

[1] Kauppila W E, Stein T S and Jesion G 1976 *Phys. Rev. Lett.* **36** 580
[2] Stein T S, Kauppila W E, Kwan C K, Parikh S P and Zhou S 1992 *Hyperfine Inter.* **73** 53
[3] Uhlmann K, Triftshäuser W, Kögel G, Sperr P, Britton D T, Zecca A, Brusa R S, Karwasz G P 1995 *Fresenius J. Analytical Chem.* **353** 594
[4] Brusa R S, Karwasz G P, Bettonte M and Zecca A1997 *Appl. Surf. Sci.* **116** 59
[5] Karwasz G P, Barozzi M, Brusa R S and Zecca A 2002 *Nucl. Instr. Meth. B* **192** 157
[6] Karwasz G P, Brusa R S, Barozzi M and Zecca A 2000 *Nucl. Instr. Meth. B* **171** 178
[7] Karwasz G P, Pliszka D, Brusa R S and Perazzolli C 2005 *Acta Phys. Pol.* **107** 666
[8] Karwasz G P, Pliszka D and Brusa R S 2006 *Nucl. Instr. Meth. B* **247** 68
[9] Karwasz G P, Pliszka D, Zecca A and Brusa R S 2005 *Nucl. Instr. Meth. B* **250** 666
[10] Karwasz G P , Brusa R S and Pliszka D 2006 *Nucl. Instr. Meth. B* **251** 520
[11] Zecca A, Sanyal D, Chakrabarti M and Brunger M J 2006 *J. Phys. B* **39** 1597
[12] Zecca A, Perazzolli C and Brunger M J 2005 *J. Phys. B* **38** 2079
[13] Zecca A, Chiari L, Sarkal A, Lima M A P, Bettega M H F, Nixon K L and Brunger M J 2008 *Phys. Rev.* **78** 042707
[14] Zecca A, Moser N, Perazzolli C, Salemi A and Brunger M J 2007 *Phys. Rev. A* **76** 022708
[15] Sullivan J P, Gilbert S J, Marler J P, Greaves R G, Buckman S J and Surko C M 2002 *Phys. Rev. A* **66** 042708
[16] Sullivan J P, Makochekanwa C, Jones A, Caradonna P and Buckman S J 2008 *J. Phys. Conf. Ser.* **133** 012004
[17] Zhang R, Faure A and Tennyson J 2009 *Physica Scripta* **80** 015301
[18] Kennerly R E 1980 *Phys. Rev. A* **21** 1876
[19] Schulz G J 1962 *Phys. Rev.* **125** 229
[20] Zubek M, Mielewska B, Channing J, King G C and Read F H 1999 *J. Phys. B* **32** 1351
[21] Sullivan J P, Gilbert S J, Buckman S J and Surko C M 2001 *J. Phys. B* **34** L467
[22] Sueoka O 1988 *J. Phys. B* **21** L631
[23] Szłuińska M, Laricchia G 2004 *Nuclear Instr. Meth. B* **221** 100
[24] Buckman S J, ICPEAC Kalamazoo invited lecture, ref. to be inserted
[25] Amarenda G, Canter K F and Schoepf D C 1996 *J. Appl. Phys.* **80** 4660
[26] Karwasz G P, Brusa R S, Piazza A and Kogel G 1995 European Community Reasearch, Project BREU-CT 90-0347, Final Technical Report, Appendix A7.1
[27] Colyert C J, Vizcaino V, Sullivan J P, Brunger M J and Buckman S J 2007 *New J. Phys.* **9** 41
[28] Dampc M, Linert I, Milosavljevic A R and Zubek M 2007 *Chem. Phys. Lett.* **443** 17
[29] Gianturco F A, Jain A and Rodriguez-Ruiz J A 1993 *Phys. Rev. A* **48** 4321
[30] McEachran R P and Stauffer A D 2009 *J. Phys. B* **42** 075202, and private information
[31] Idziaszek Z and Karwasz G P 2006 *Phys. Rev. A* **73** 064701
[32] Gribakin G and Ludlov J 2004 *Phys. Rev. A* **70** 032720 and private information, see Karwasz G P, Brusa R S, Pliszka D, Idziaszek Z, Nowakowska H 2006 *Acta Phys. Pol.* **110** 605
[33] Karwasz G P, Karbowski A, Idziaszek Z, Brusa R S 2008 *Nucl. Instr. and Meth. B* **266** 471
[34] Sueoka O, Makochekanwa C, Tanino H and Kimura M 2005 *Phys. Rev. A* **72** 042705
[35] Utamuratov R, Kadyrov A S, Fursa D V and Bray I, XV ICPEAC, Kalamazoo, https://www.icpeac2009.physics.wmich.edu/webpdffiles/Fr126.pdf, to be inserted
[36] Kawasz G P 2005 *Eur. Phys. J. D* **35** 267; Karwasz G P 2006 *Eur. Phys. J. D* **37** 153
[37] Gianturco F A, Mukherjee T and Occhigrossi A 2001 *Phys. Rev. A* **64** 032715
[38] Baluja K L, Zhang R, Franz J and Tennyson J 2007 *J. Phys. B* **40** 3515
[39] Ingr M, Polášek M, Čarsky P and Horáček J 2000 *Phys. Rev. A* **62** 032703
[40] Machado L E, Mu-Tao L, Brescansin L M, Lima M A P and McKoy V 1995 *J. Phys. B* **28** 467
[41] Karwasz G P, Zecca A and Brusa R S 2001 *Riv. Nuovo Cim.* **24** 1
[42] Čurík R, Ziesel J P, Jones N C, Field T A and Field D 2006 *Phys. Rev. Lett.* **97** 123202
[43] Humberston J W 1978 *J. Phys. B* **11** L343
[44] Beale J, Armitage S and Laricchia G 2006 *J. Phys. B* **39** 1337