Positron scattering on benzene and cyclohexane: Experiment and modified effective range theory

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Abstract. Total cross sections for positron scattering on benzene and cyclohexane measured with high angular resolution in the 0.5–20 eV range are compared with previous experimental data. Present data showing a rise in the zero energy range agree much better with the theory than previous experiments. The rise can be reproduced by the modified effective range theory, using three partial waves.

1 Introduction

Positrons, as compared to electrons, are an alternative probe in testing both quantum mechanics models as the atomic structure (see [1] for a more extended comparison). In brief, positrons are not subject to Pauli's principle, so they can explore the atomic space also in regions forbidden for electrons. In our previous measurements for argon, molecular nitrogen and hydrogen [2] we showed the total cross sections rise in the zero-energy limit for all these targets, but in the region of a few eV remain constant up to the positronium-formation threshold. However, theories find it difficult to explain this behavior, disagreeing even on the very existence of Ramsauer-Townsend's minimum for these targets (see [2] for detailed discussion).

Modified effective range theory MERT [3] developed in 60'ies for electron scattering in the low energy region has been recently applied for positron scattering on Ar and N_2 [4], allowing to extrapolate the experimental total cross section data to the zero energy limit. The main difference of that novel approach [4] with previous MERT approximations is that we obtained the phase shifts directly from the analytical solution of Schrdinger equation with the polarization potential, instead of using their approximate series.

In this paper we compare our total cross sections for positrons scattering on two organic molecules, benzene and cyclohexane, with recent measurements from Tokyo group for benzene [5–8] and cyclohexane [9]. Present experimental data have been obtained with a higher angular resolution precision (thanks to lower magnetic fields used and smaller scattering call apertures) than the data from Tokyo. Differently from those latter, present data show a rise in the low energy limit, in agreement with the *ab-initio* theory [10]. In the theoretical part of the paper we extend the previous MERT analysis [4] to the two highly polarizable targets (dipole polarizability being 10.54 $Å^3$ for benzene and 10.95 $Å^3$ for cyclohexane, comparing to 1.64 $Å^3$ for Ar and 1.74 $Å^3$ for N_2).

2 Experiment

The apparatus for positron scattering uses a ^{22}Na compact radioactive positron source, 1μm thin W-monocrystal moderator, an electrostatic extraction and optical system, a 90° bend for discrimination of fast positrons, and magnetically guided (by 9 G longitudinal field) injection system to the scattering cell (10 cm long with 1.5 mm diameter entrance and exit apertures). The total cross section σ have been obtained by measuring the attenuation rate of the transmitted positron current, according to the standard de Beer-Lambert's formula

$$I = I_0 \ exp \ (-pl\sigma/kT) \tag{1}$$

where l is the length of the scattering cell, p is the gas pressure, T is temperature of the gas and k is Boltzmann's constant. I and I_0 stand for positron currents measured with and without gas in the scattering cell, respectively.

The absolute pressure in the scattering cell, the temperature and positron paths in the scattering cell were evaluated with 5%, 1% and 0.5% precisions, respectively. However, the main source of systematic error (possibly underestimating the cross section) is the thermal transpiration [11] due to non-perfect equilibrium of pressure in the scattering cell and the pressure gauge. However, this error in the worst case (assuming the validity of laminar flow and Knudsen's formula) does not exceed 3% in our measurements. Details of the apparatus, measurement procedures and the error analysis have been presented in our previous papers [2,12].

3 Comparison with previous experiments and theory

For benzene our data agree very well with the early data by Sueoka [13] who performed a careful analysis of the magnetic field on the systematic error leading to underestimation of the cross sections. For his tabulated data he chose measurements with the lowest field (4.5 G) in the low energy data. For our knowledge, successive data from the same data were performed with similar (6–8 mm diameter) apertures in the scattering cell but with higher magnetic fields (9 G). Moreover, at the very first glance the low energy maximum in data from ref. [5,8], see Fig. 1, resemble structures already observed in the paper of Sueoka [13] but with higher magnetic fields.

As shown in our previous paper [2], also for nitrogen the data from Tokyo lab were systematically lower than other measurements in particular those from the Detroit lab [14], with the difference rising with lowering energy. In the paper [2] we gave a detailed analysis, using theoretical differential cross sections [15]. Those data allowed us to quantify the error due to an incomplete screening against scattered positrons: the longitudinal magnetic field re-captures positrons scattered in forward angles and guide them to the detector. This lowers the measured cross section. In the limit case, for 9 G field, 8 mm diameter scattering apertures and 1.14 eV collision energy, all positrons scattered into angles below 90° are guided to the detector. For 4 eV collision energy, all positrons scattered below 30° are collected by the detector if 8 mm diameter apertures are used; for a uniform angular distribution a possible error would be 15%. At 1 eV order energies a possible error can be by several folds, see [2]. In Fig. 1 and 2 we see such a diverging difference for all three gases (N_2, C_6H_6, C_6H_{12}) starting below 4–5 eV.

The only dedicated theoretical paper we are aware on benzene is that by Occhigrossi and Ginaturco [10] in which a parameter-free, single-centre expansion of their own model (static, polarization and correlation) potential was used; we are not aware of any results for cyclohexane. Data of ref. [10] indicate a rise in the total cross section, similarly to the present experiment and that by Sueoka [13] but are somewhat lower. On the other hand, the "muff-in" model

by Kimura et al. [7] agree perfectly with their own experiment but does not contain enough details to evaluate its theoretical consistency. We stress that calculations by Occhigrossi and Gianturco [10] agree very well for ethene and acetylene with Tokyo data, but again in the early edition [16].

4 Modified effective range theory in the analytical solution

We have noticed already in our preliminary paper [1] that cyclohexane cross sections in the low energy limit follow a MERT-like dependence; however we were able to use only a phenomenological fit, with no physical explanation for it. Here, we analyze the low-energy regime using MERT with exact solutions of the Schrödinger equation for the long range part of the interaction potential [4]. This allows us to extrapolate the experimental cross-section data to the limit of zero energy and to determine the value of the s-wave scattering length.

At large distances the interaction between positrons and a molecule is given by the polarization potential $-\alpha e^2/2r^4$, where α is the dipolar polarizability. The Schrödinger equation for such a potential can be solved exactly (see [4] and reference therein). The solutions are scaled by the characteristic distance $R^* = (\alpha e^2 \mu/\hbar^2)^{1/2}$ and 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.
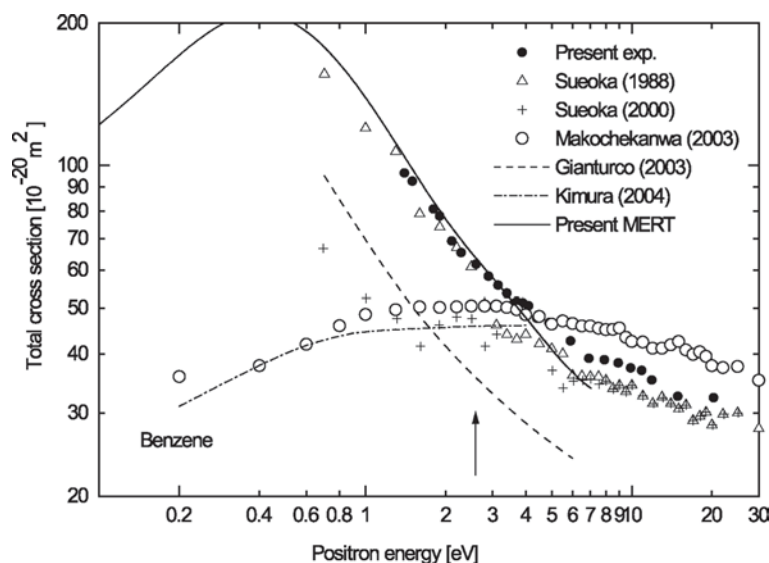

Fig. 1. Total cross sections for positron scattering on benzene. Experimental: triangles, Sueoka, Ref. [13], experiment with 4.5 G field in the low energy limit, crosses, Sueoka et al., Ref [5]; circles, Makochekanwa et al., Ref. [6], experiment with 9 G field, identical data with those from Ref. [7]. Theory: Occhigrossi and Gianturco, Ref. [10], parametr-free, single-centre expansion; Kimura et al, Ref. [7] "muff-in" model; present MERT model with 5 parameter fit. The arrow indicates the positronium-formation threshold.

In present MERT analysis we consider the range of energies up to 16 E^*, 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 [4] for details). In contrast, the phase shifts for l ≤ 2 are calculated from the exact formulas for r^{-4} potential [4], where for the short range parameter $B_l = \tan(\phi_l + \pi/2)$ 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 $B_l(0), R_l$, 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 and cyclohexane, in Figs. 1 and 2, respectively. We have applied 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 the reliable value of this parameter. The fitting parameters and the values of R^* and E^* are presented in Table I.
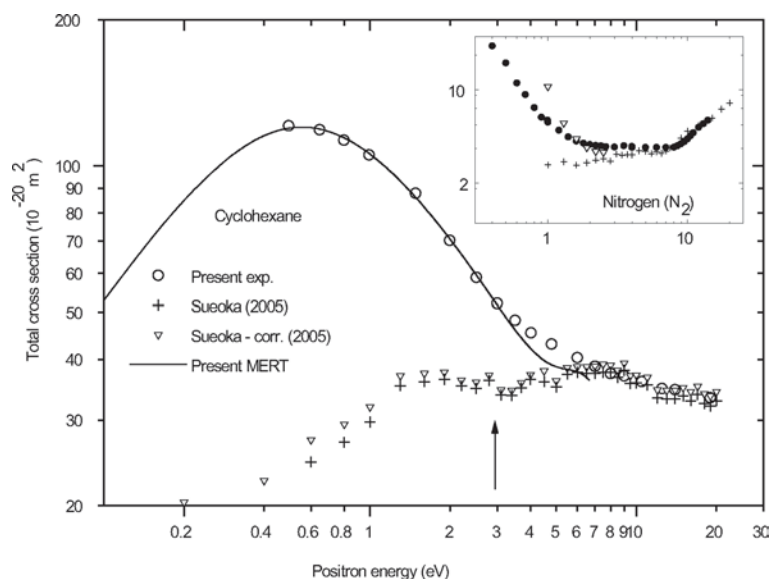

Fig. 2. Total cross sections for positron scattering on cyclohexane. Experimental: crosses Sueoka, Ref. [9], experiment with 9 G field, and 6 mm scattering call apertures diameter; triangles. The same data corrected for the angular resolution error, Ref. [9]. Theory: present MERT model with 5 parameter fit. The arrow indicates the positronium- formation threshold.

Table 1. The characteristic distance R^*, characteristic energy E^*, and five fitting parameters: 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 wave) for benzene and cyclohexane.

	$R^*(a_0)$	$E^*(eV)$	a/R^*	R_0/R^*	$B_1(0)$	R_1/R^*	$B_2(0)$
C_6H_6	8.34	0.195	0.30	0.02	0.77	0.20	6.92
C_6H_{12}	8.57	0.185	−0.08	0.68	2.40	−0.15	−1.23

The present MERT approach predicts that the total cross-section for both targets show a maximum at low energies; however, the position of this maximum is beyond the range of the available data, and its existence cannot be verified by comparison with the experiment (therefore we truncated the energy scale for both targets at 0.1 eV). We would like to stress

that the lack of data for sufficiently low energies ($E < 2E^*$), may lead to significant errors in determination of the scattering length. Moreover, the large size of molecules, comparable to R^*, can introduce some important modifications of r^{-4} interaction at distances of the order of R^*. This can be accounted, for example, by introducing higher order terms in the expansion of short-range parameter $B_l(k)$.

5 Conclusions

Present experimental data for benzene agree with the early measurements by Sueoka [13] in which, in the course of the experiment he carefully evaluated the influence of the magnetic field on the "angular resolution" error and published data with the low field used. Successive papers from that group do not give details of the two crucial elements needed to evaluate the "angular resolution" error, i.e. the magnetic field and the scattering cell apertures. Therefore, we were able to quote a possible error only in the case of nitrogen, using our previous analysis [2] of Sueoka and collaborators data. This analysis, based on simple considerations on the cyclotron radius of projectile positrons indicate that in the case of combined strong fields (of 10 G order) and large apertures (of few mm radius) a possible underestimation of the cross section can be by few folds at 1 eV. This would explain disagreement between present and Tokyo data both for cyclohexane and benzene data.

Present MERT analysis shows that the low energy rise of the cross sections can be explained using only three partial waves. However, the lack of data in the very low energy regime does not allow to perform this analysis with the sufficient certainty on the fitting parameters. In particular, even the very sign of the scattering length (i.e. the existence or not of the Ramsauer's minimum) is uncertain. The difference between the fit and the experiment above the positronium formation threshold indicates that MERT analysis can be successfully used for the partitioning analysis, even for such big targets like benzene and cyclohexane.

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