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Positron annihilation in benzene, aniline and cyclohexane

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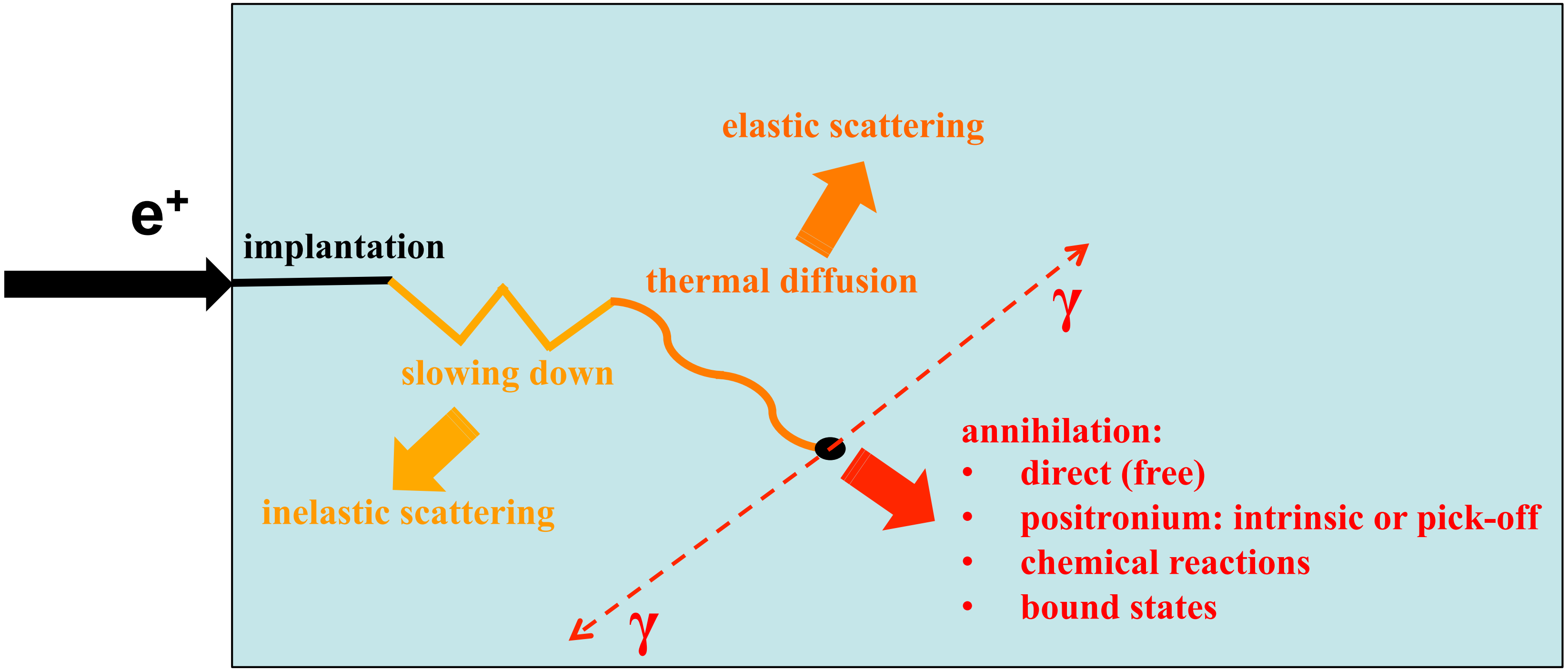
What is it about?



e^+

implantation

slowing down

inelastic scattering

thermal diffusion

elastic scattering

γ

γ

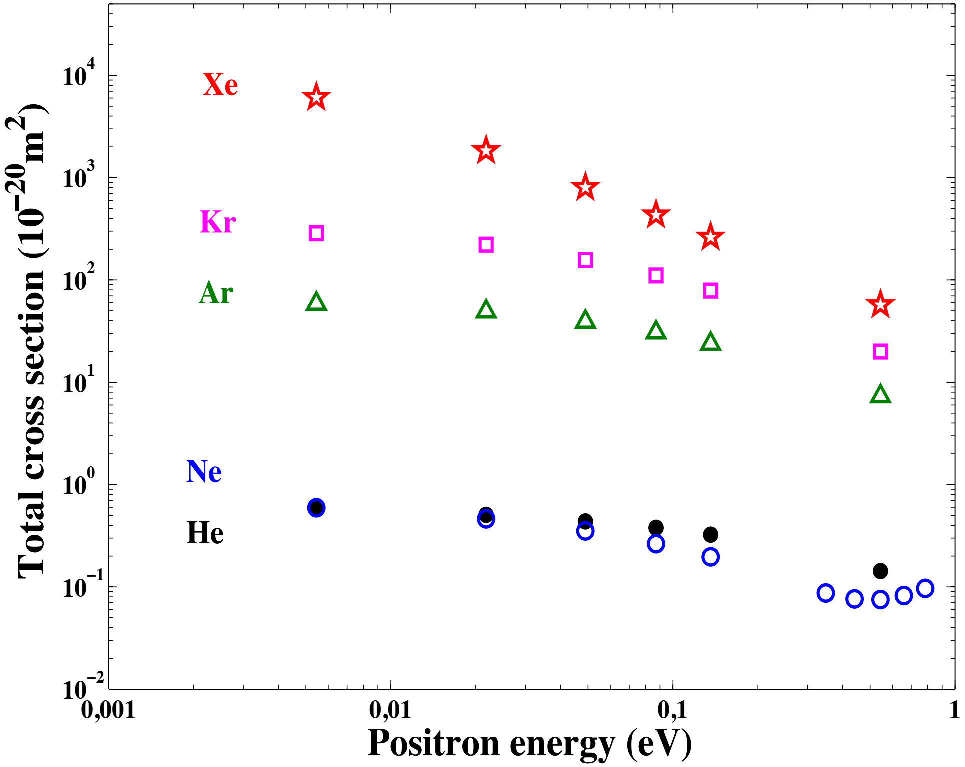
annihilation:

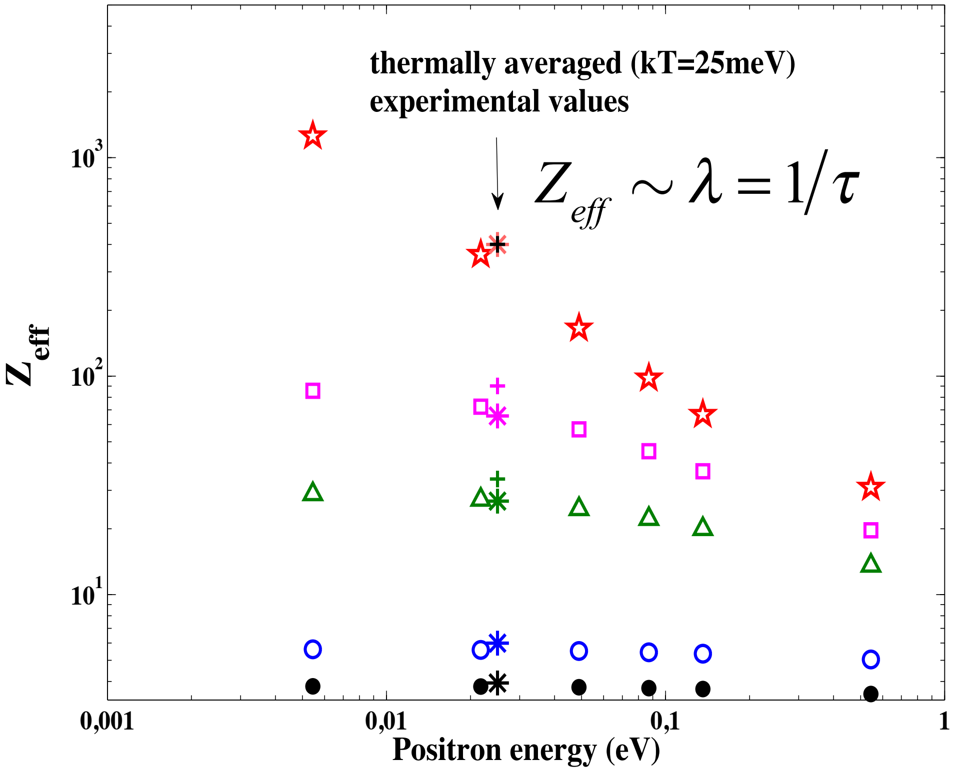
- direct (free)
- positronium: intrinsic or pick-off
- chemical reactions
- bound states

The primary goal of this study is to find any qualitative or quantitative links between single positron-molecule collisions quantified by ***cross sections*** measured in a gas phase and ***annihilation rates*** measured in condensed phase of matter for large molecules.

Positron direct annihilation vs elastic scattering cross-section

low-pressure noble gases at room temperature





Theoretical data („many body theory") from D. G. Green, J. A. Ludlow and G. F. Gribakin, Phys. Rev. A 90, 032712 (2014)

Experimental data from:

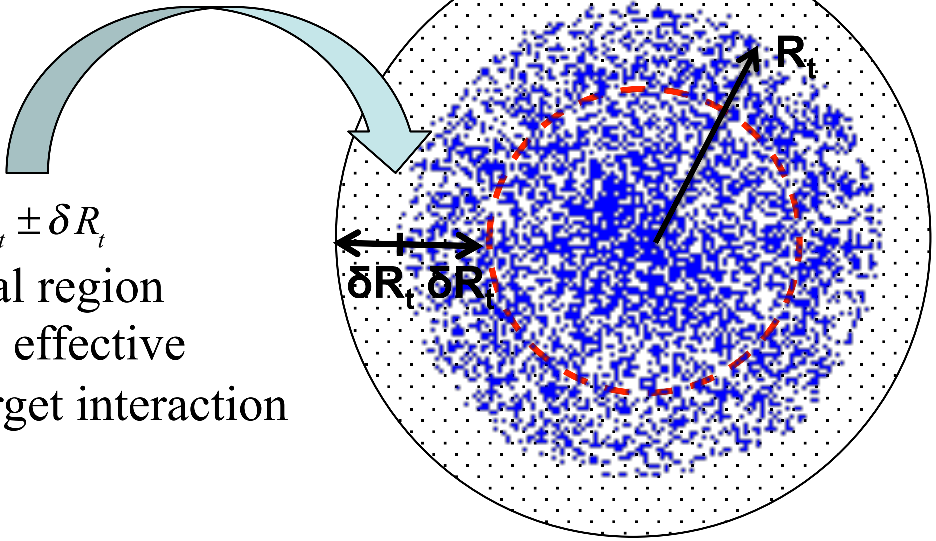
- P. G. Coleman, T. C. Griffith, G. R. Heyland, and T. L. Killeen, J. Phys. B: At. Mol. Phys. 8, 1734 (1975)
- T. J. Murphy and C. M. Surko, J. Phys. B: At., Mol. Opt. Phys. 23, L727 (1990)
- G. L. Wright, M. Charlton, T. C. Griffith, and G. R. Heyland, J. Phys. B: At. Mol. Phys. 18, 4327 (1985)
- T. C. Griffith and G. R. Heyland, Phys. Rep. C 39, 169 (1978)
- K. Iwata, R. G. Greaves, T. J. Murphy, M. D. Tinkle, and C. M. Surko, Phys. Rev. A 51, 473 (1995)

Positron direct annihilation vs scattering cross-section

Two-body interaction with noble gases and simple molecules

$$\boxed{Z_{eff}(k) = F\left(R_t^2 + \frac{\sigma_{el}(k)}{4\pi} + \frac{R_t}{k}\sin\left[2\eta_0(k)\right]\right)}$$

G. F. Gribakin, Phys. Rev. A 61, 022720 (2000)



$R_t \pm \delta R_t$
spatial region
of the effective
positron-target interaction

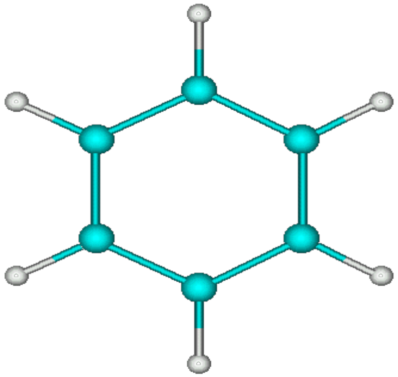
$$Z_{eff} \sim \lambda = 1/\tau$$

σ_{el} - elastic scattering cross section

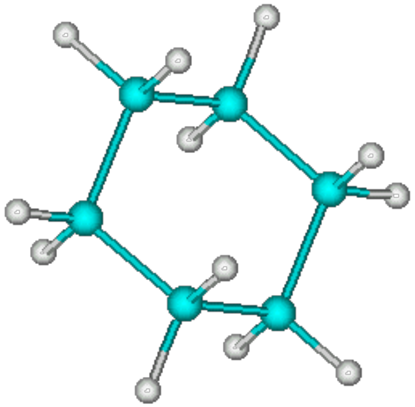
η_0 - *s*-wave scattering phase-shift

Subjects of present investigation

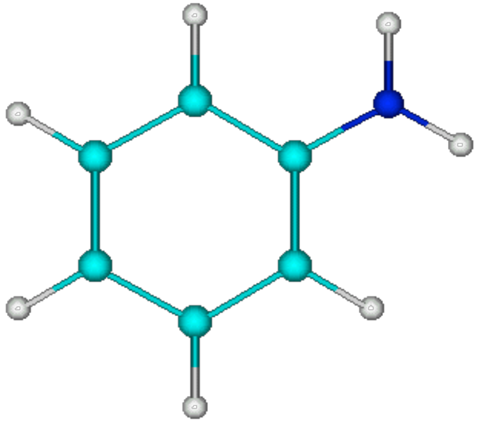
Benzene C_6H_6



Cyclohexane C_6H_{12}



Aniline $C_6H_5NH_2$



Dipole polarizabilities:

$\alpha \approx 70.9\ [a_0^3]$

$\alpha \approx 73.8[a_0^3]$

$\alpha \approx 81.7[a_0^3]$

Permanent dipole moments:

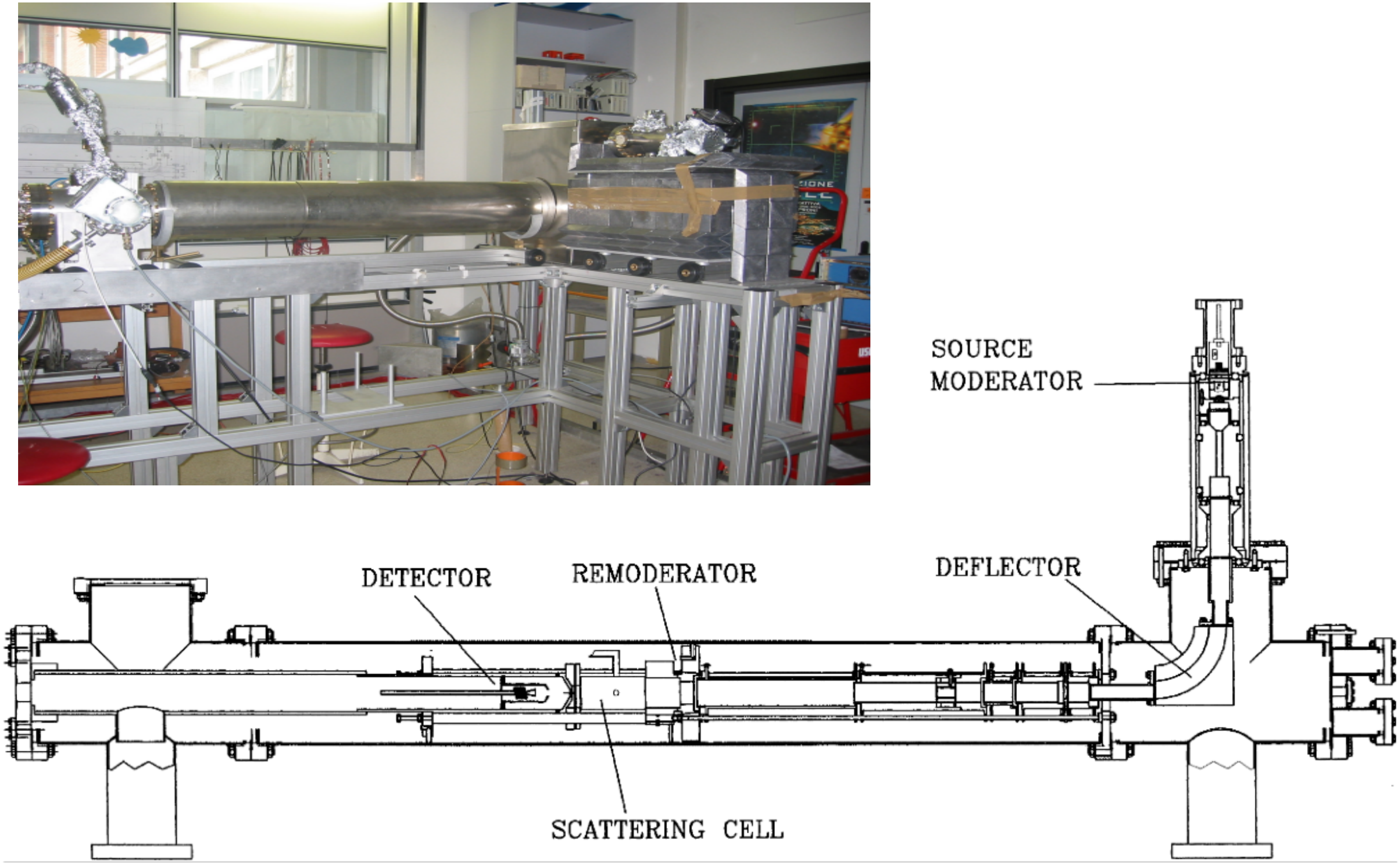
$M \approx 0$ [D]

$M \approx 0$ [D]

$M \approx 1.13$ [D]

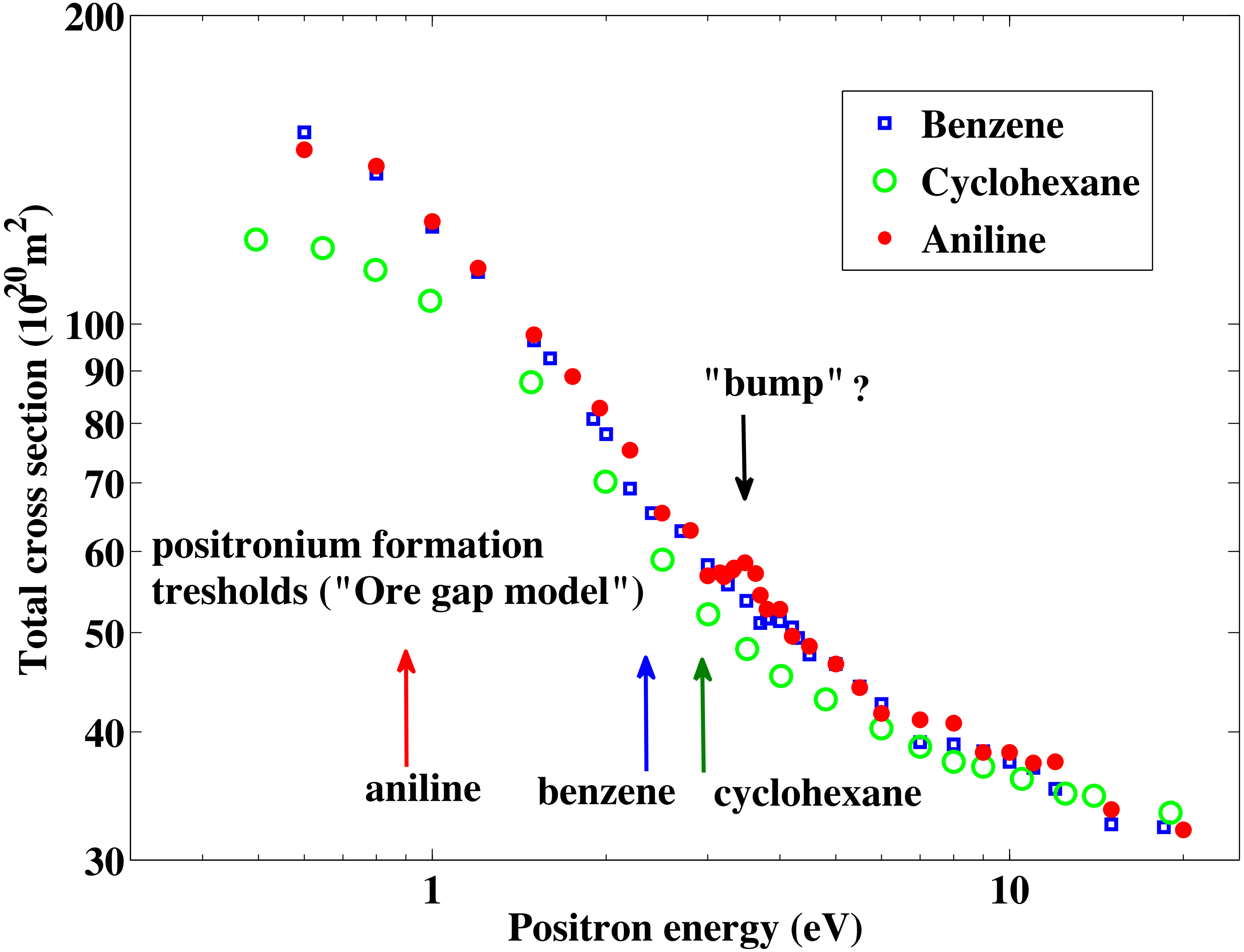
CRC Handbook of chemistry and physics, ed. 86 (2005)

Trento low-energy gas-phase positron beam experiments



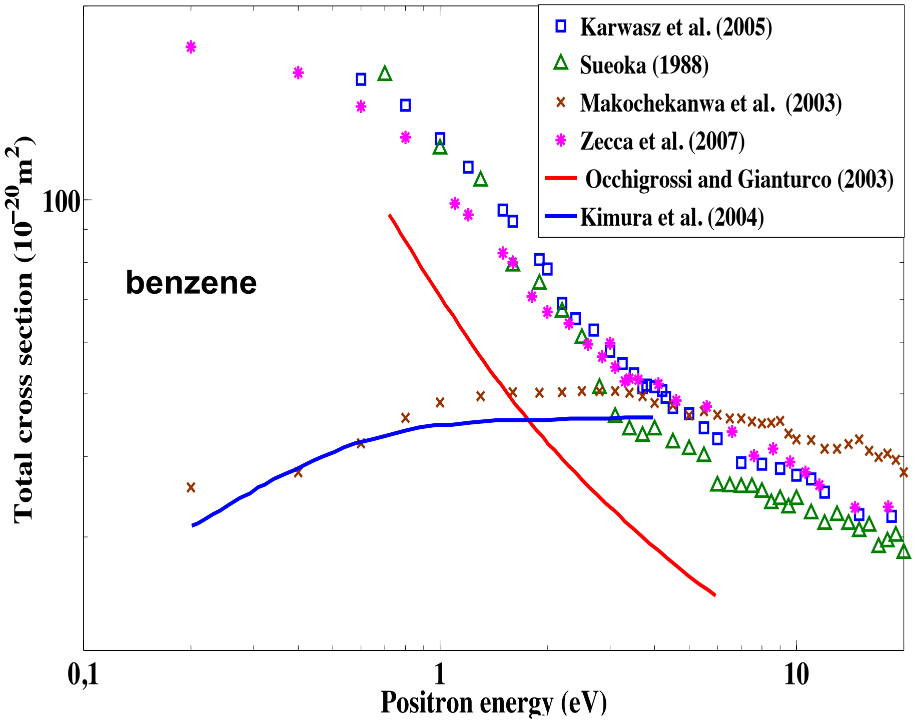
G. P. Karwasz, R.S. Brusa, M.Barozzi and A.Zecca, Nuclear Instr. and Methods in Physics B 171, 178 (2000)

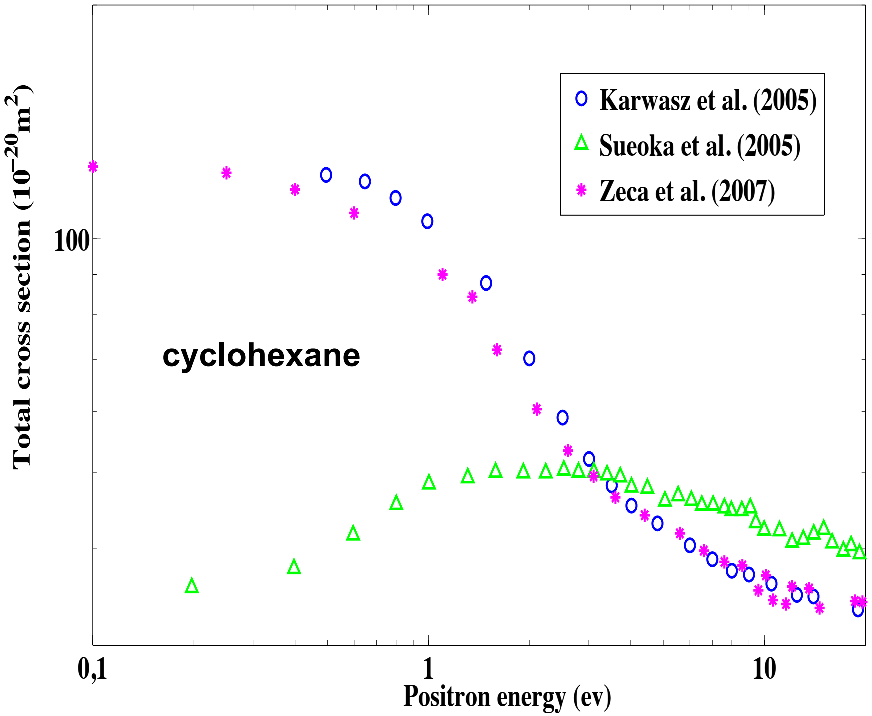
Total cross-section for positron scattering from benzene, cyclohexane and aniline in a gas phase

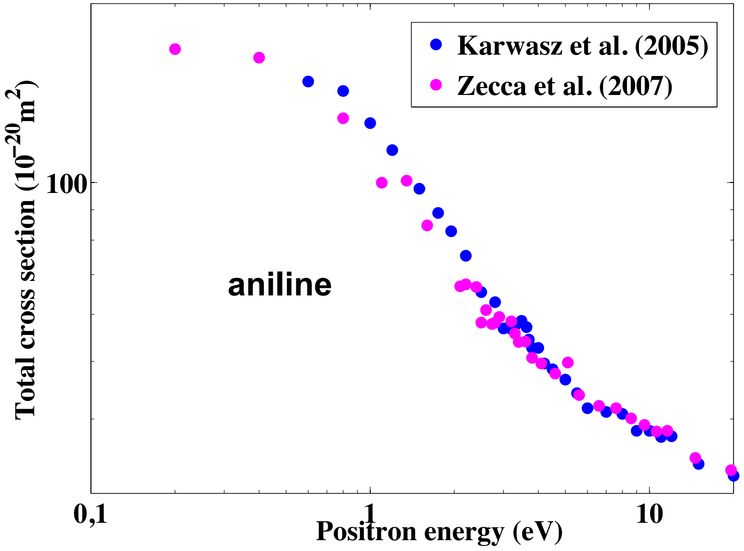


G.P. Karwasz, D. Pliszka, R.S. Brusa, C. Perazzolli, Acta Phys. Pol. 107, 666 (2005)

Total cross-sections in the literature for C_6H_6, C_6H_{12} and $C_6H_5NH_2$

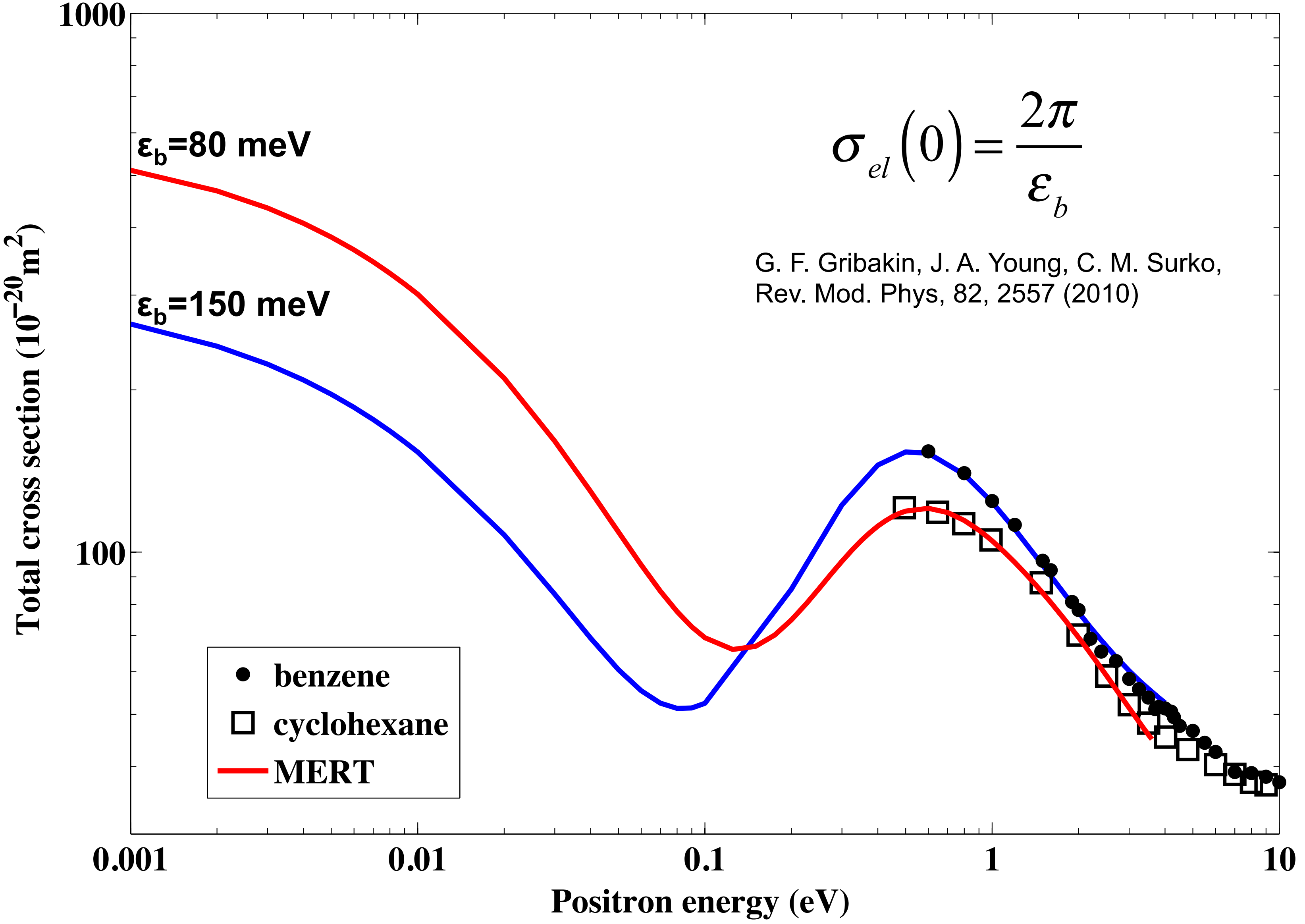






Extrapolation of total cross-section down to thermal energies by Modified Effective Range Theory (MERT)

(K. Fedus, G. Karwasz, Z. Idziaszek, Phys. Rev. A. 88, 012704 (2013))



Anomalous annihilation rates for large molecules in a gas phase

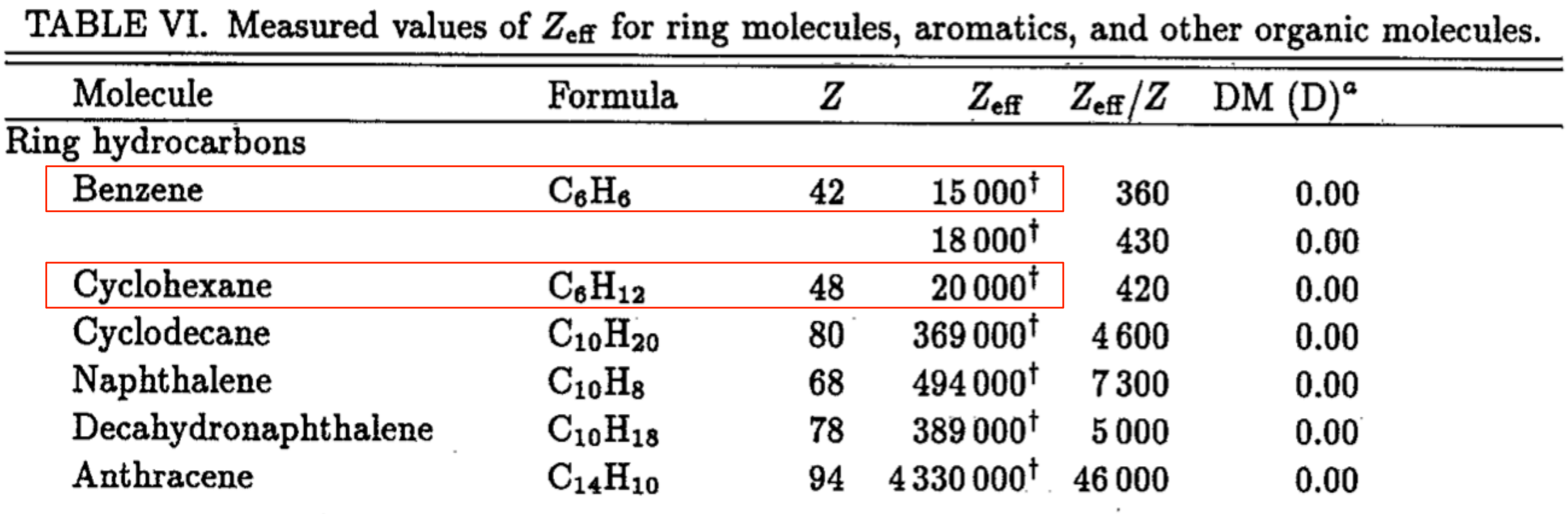
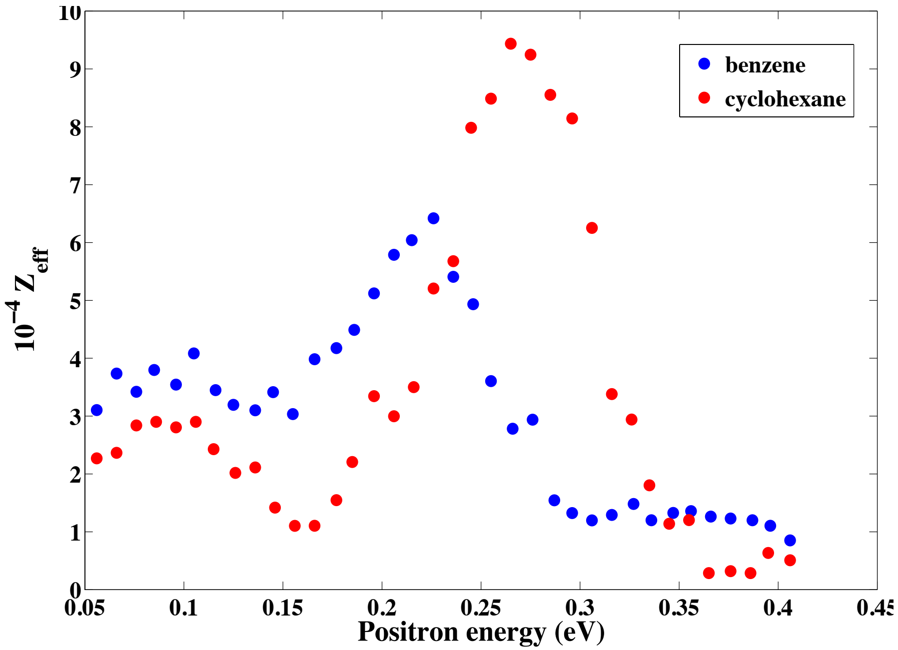


TABLE VI. Measured values of Z_{eff} for ring molecules, aromatics, and other organic molecules.

Molecule	Formula	Z	Z_{eff}	Z_{eff}/Z	DM (D)[a]
Ring hydrocarbons					
Benzene	C_6H_6	42	15 000†	360	0.00
			18 000†	430	0.00
Cyclohexane	C_6H_{12}	48	20 000†	420	0.00
Cyclodecane	$C_{10}H_{20}$	80	369 000†	4 600	0.00
Naphthalene	$C_{10}H_8$	68	494 000†	7 300	0.00
Decahydronaphthalene	$C_{10}H_{18}$	78	389 000†	5 000	0.00
Anthracene	$C_{14}H_{10}$	94	4 330 000†	46 000	0.00

K. Iwata, R. G. Greaves, T. J. Murphy, M. D. Tinkle, and C. M. Surko "Measurements of positron-annihilation rates on molecules" Phys. Rev. A 51 (1995), pp. 473-87.



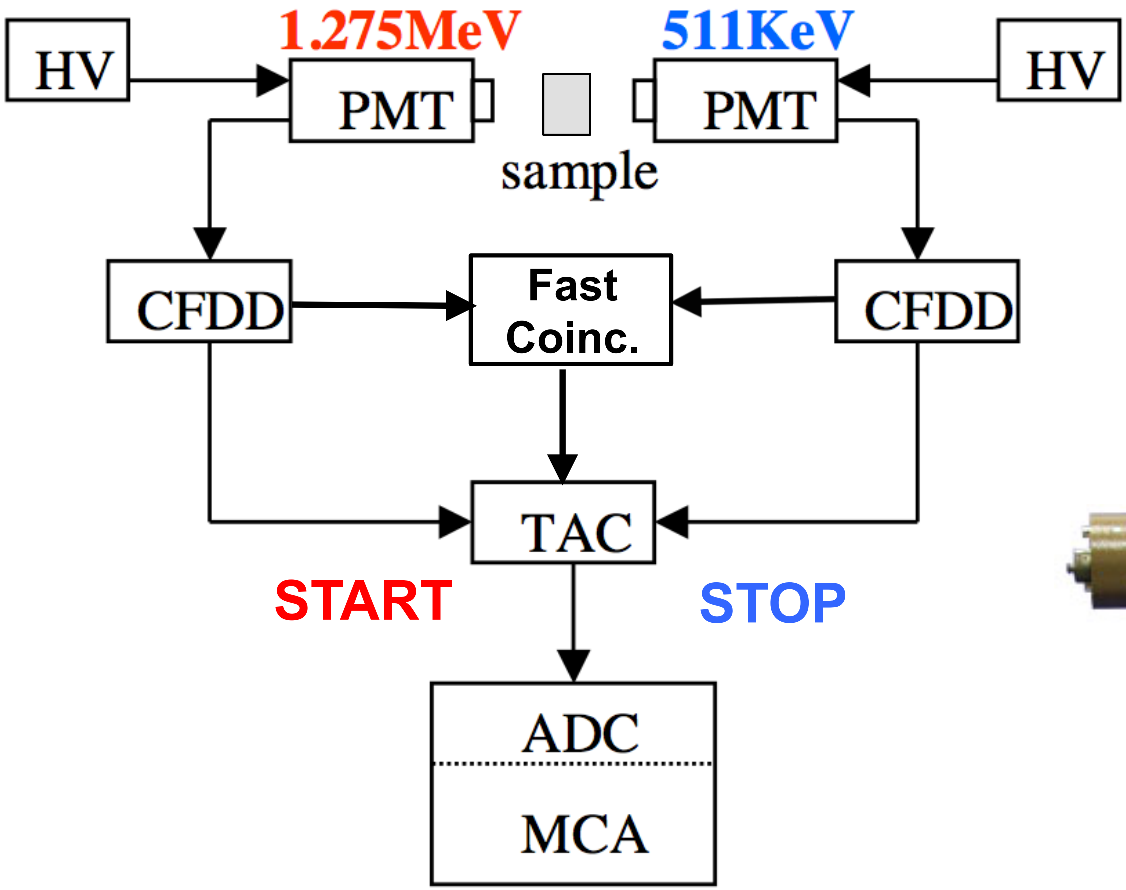
thermally averaged $\langle Z_{\mathrm{eff}} \rangle$ at 300K:

$C_6H_6 \sim 15000 \quad < \quad C_6H_{12} \sim 20000$

Positron Annihilation Lifetime (PALS) Measurements

in liquid phase at room temperature

ORTEC PALS FAST-FAST COINCIDENCE SYSTEM



HV

1.275MeV

PMT

sample

511KeV

PMT

HV

CFDD

Fast Coinc.

CFDD

TAC

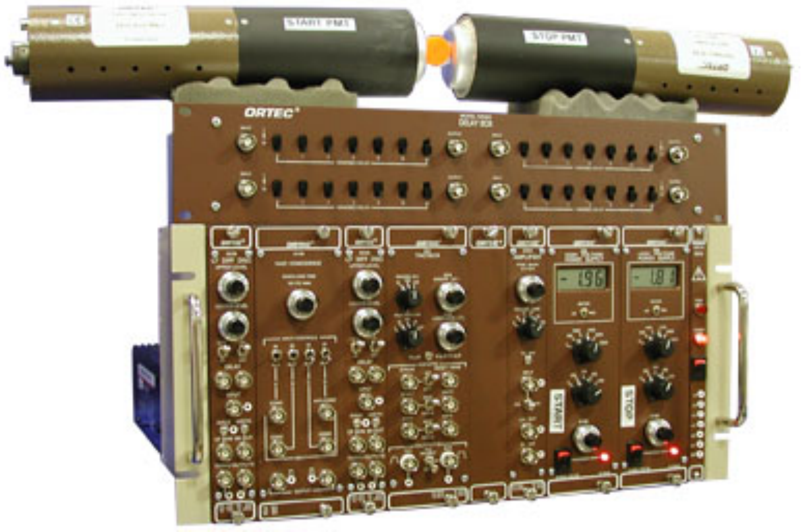
START

STOP

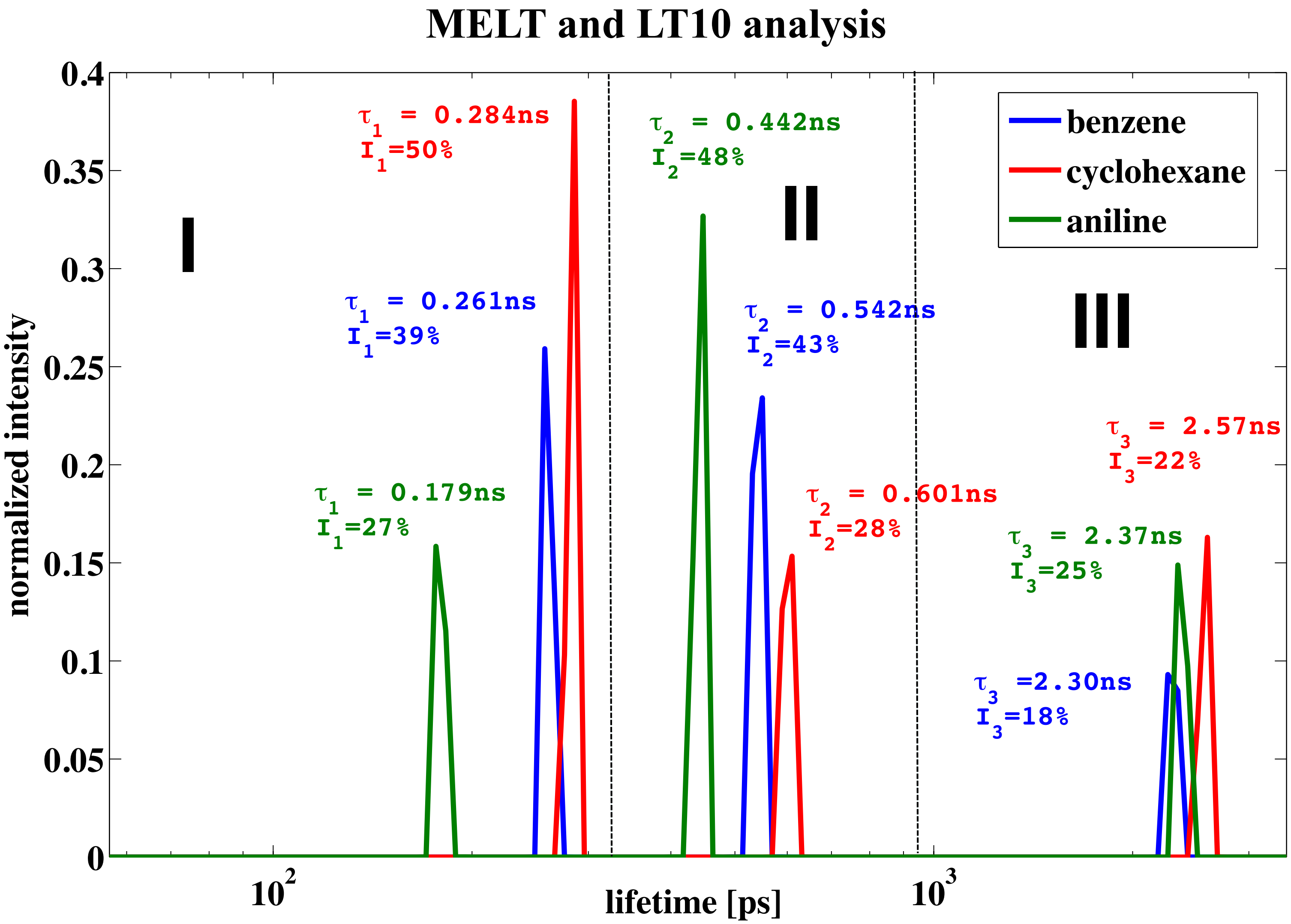
ADC

MCA

- ^{22}Na source in 7*μm* thick kapton foil with 10*μCi* activity
- 180*ps* system resolution
- 3 acquisitions per sample
- >10^6 counts per acquisition



PALS results for liquid C_6H_6, C_6H_{12} and $C_6H_5NH_2$

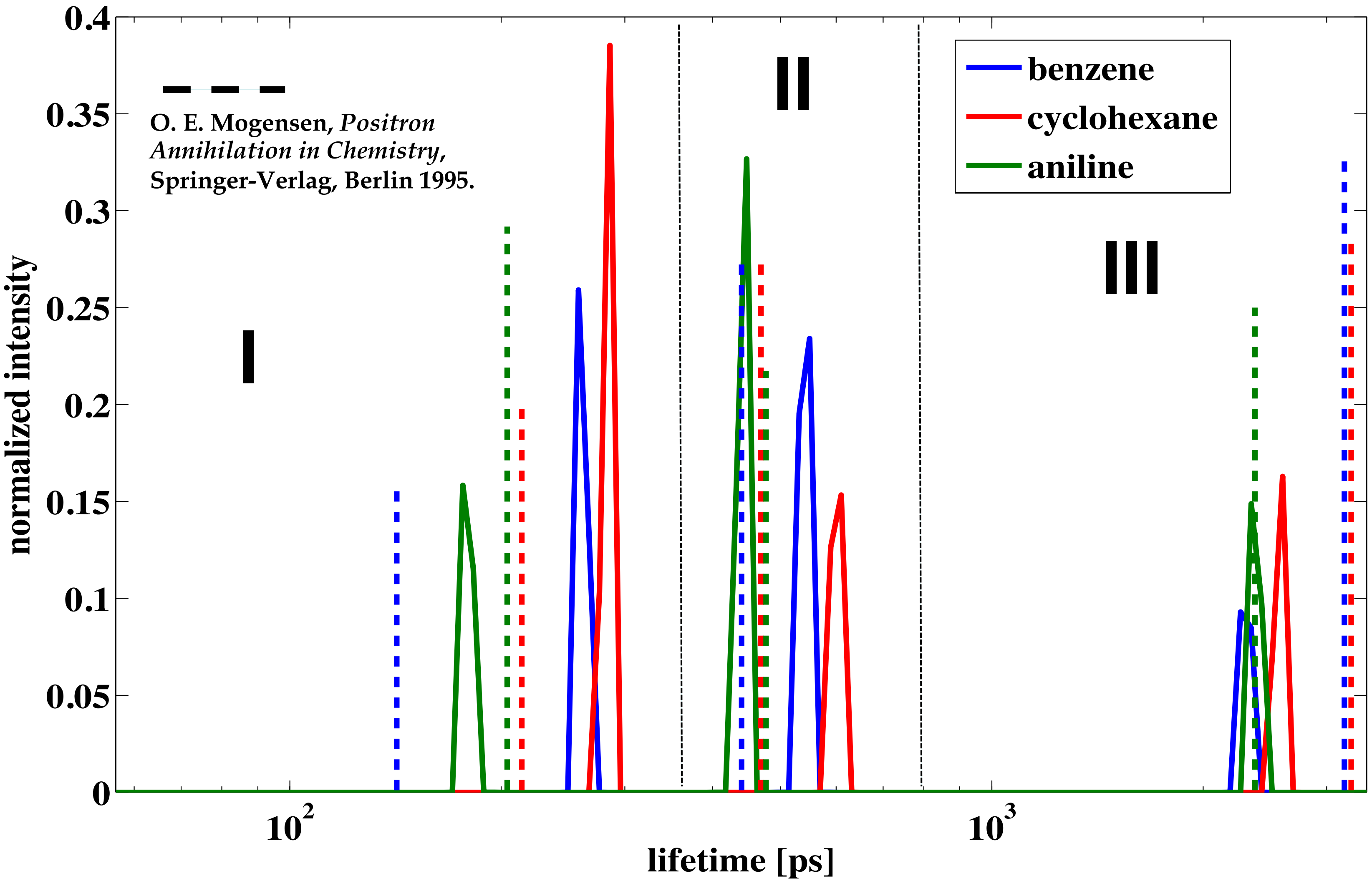


τ_1 - para-positronium
and other fast intristic processes

τ_2 – direct annihilation

τ_3 - ortho-positronium

PALS results for liquid C_6H_6, C_6H_{12} and $C_6H_5NH_2$

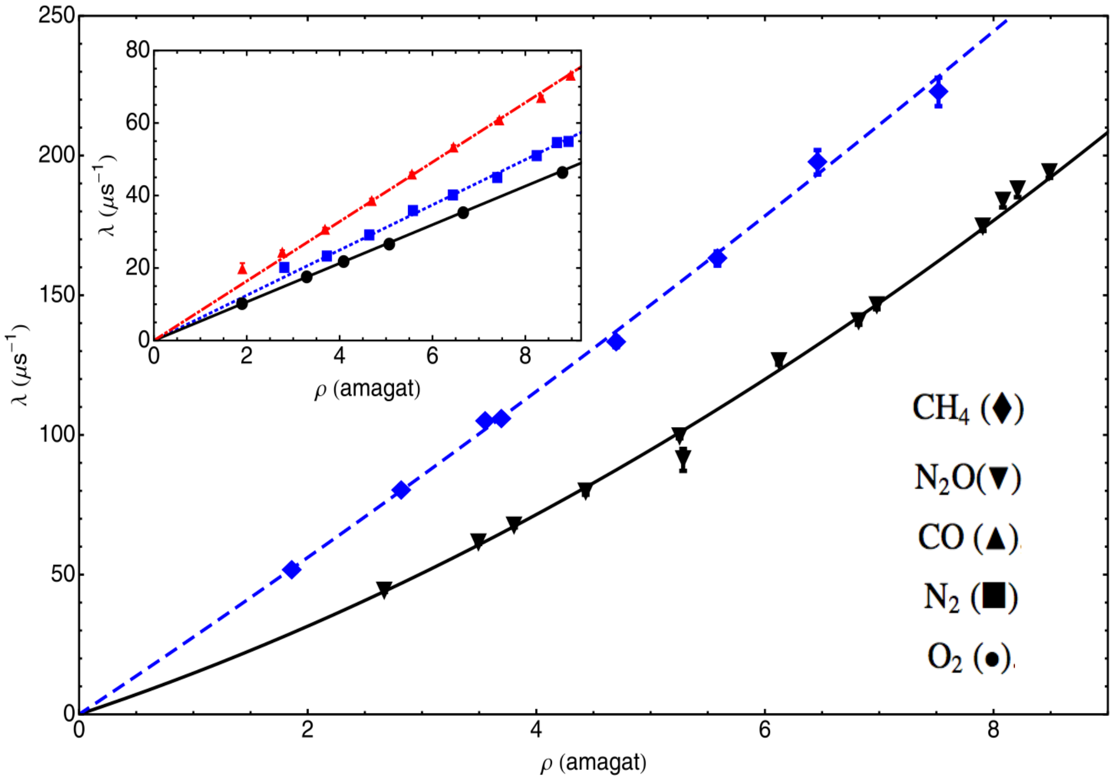

O. E. Mogensen, *Positron Annihilation in Chemistry*, Springer-Verlag, Berlin 1995.

τ_1 - para-positronium
and other fast intristic processes

τ_2 – direct annihilation

τ_3 - ortho-positronium

Complex behaviour of annihilation rates in condensed matter



M Charlton, T Giles, H Lewis and D P van der Werf, J. Phys. B: At. Mol. Opt. Phys., 46, 195001 (2013)

- Spur models
- Ore gap models
- Blob models

…

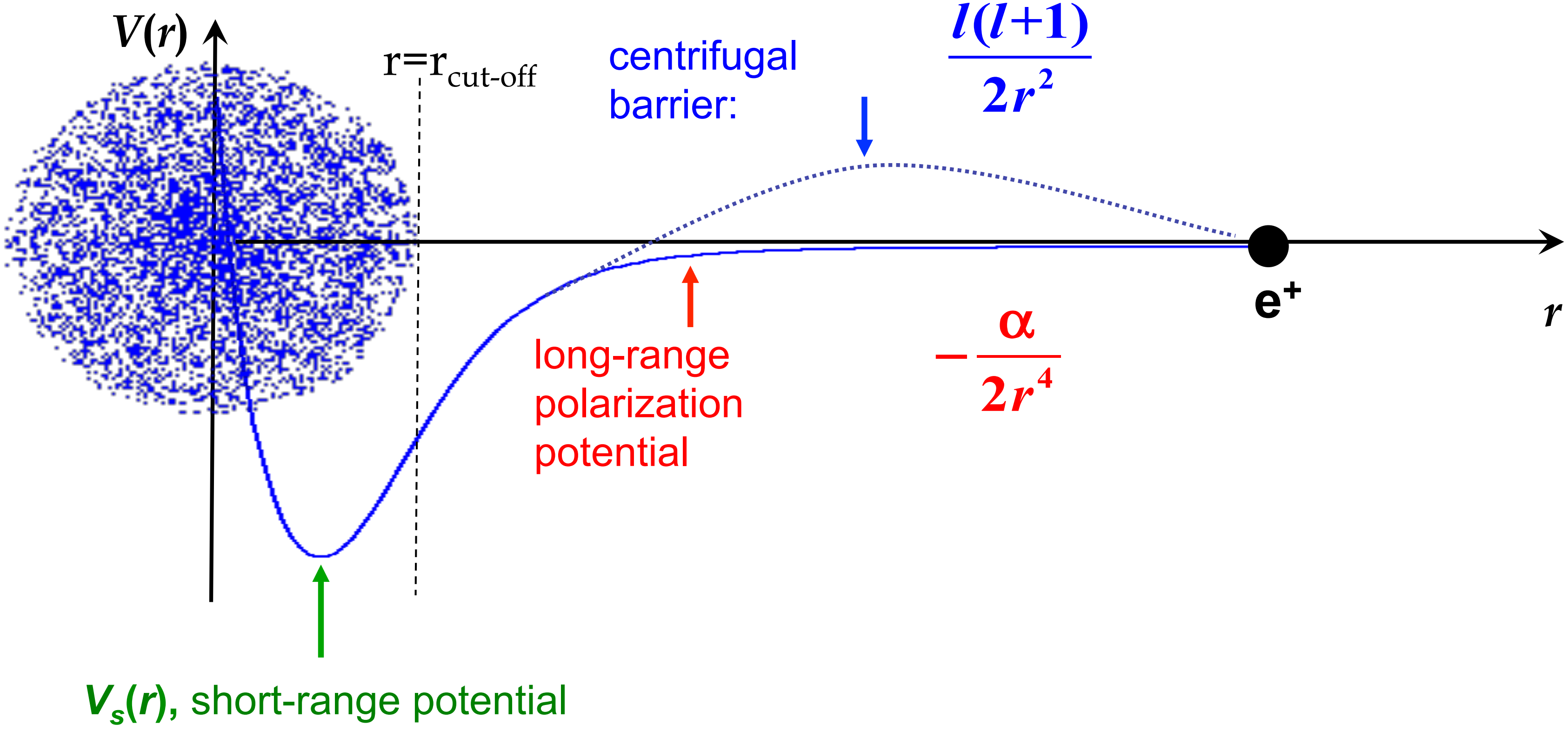
New advanced positron chemistry models are needed in order to describe how the multi-body interaction in condesned matter distorts the character of single positron – molecule interaction.

Thank you for your attention

Toruń, Poland

Extrapolation of total cross-section down to thermal energies by Modified Effective Range Theory (MERT)

$$\boxed{\left[-\frac{1}{2}\frac{d^2}{dr^2}+\frac{l(l+1)}{2r^2}-\frac{\alpha}{2r^4}-V_S(r)-E\right]rR_l(k,r)=0}$$



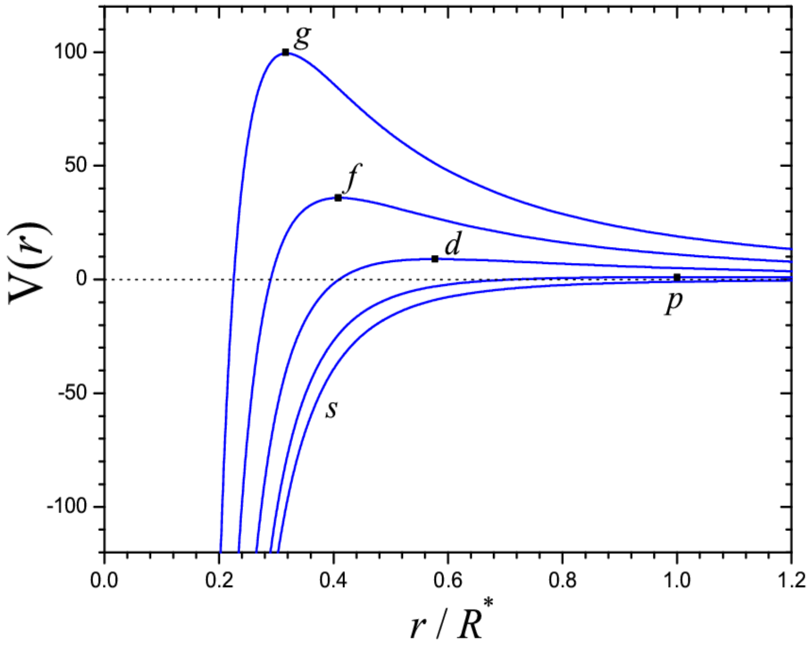
Scattering on polarization potential

Mathieu differential equation:

$$\left[\frac{d^2}{dr^2}-\frac{l(l+1)}{r^2}+\frac{\left(R^*\right)^2}{r^4}+k^2\right]\Phi_l(r)=0$$

$R^*=\sqrt{\alpha}$ - characteristic range of r^4 interaction

T. F. O'Malley et al. J. Math. Phys. 2, 491 (1961)



Behavior of the solution at large *r*

$$\Phi_l(r)\underset{r\to\infty}{\sim}\sin\left(kr-\frac{1}{2}l\pi+\eta_l\right)$$

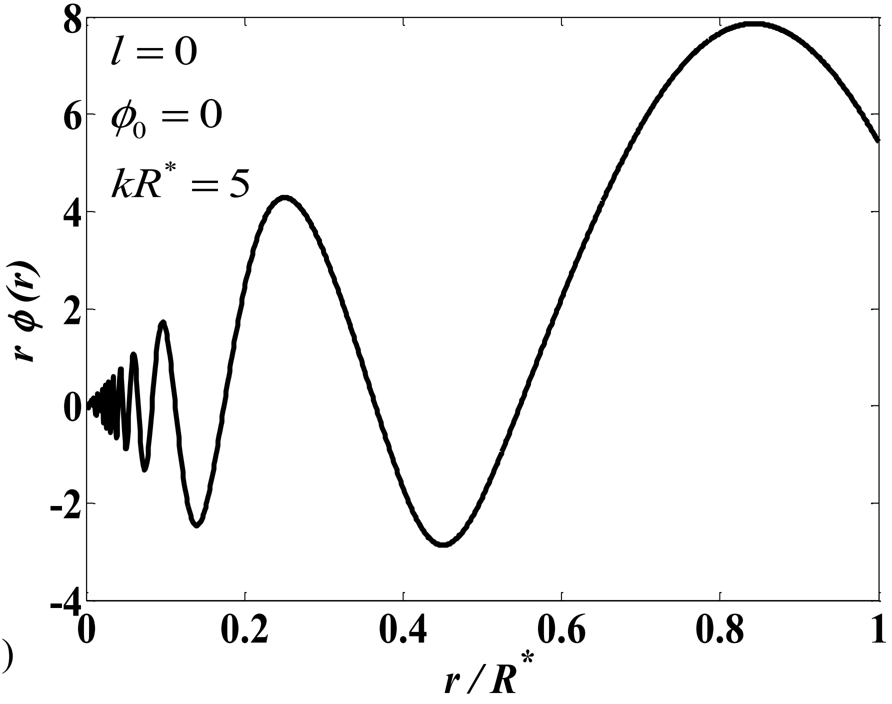
total phase shift: η_l

Behavior of the solution at small *r*

$$\Phi_l(r)\underset{r\to 0}{\sim}r\sin\left(R^*/r+\phi_l\right)$$

short-range phase: ϕ_l

Z. Idziaszek and G. Karwasz, Phys. Rev. A 73, 064701 (2006)



Scattering phase shift

$$\tan\eta_l = \frac{m_l^2 - \tan^2\delta_l + \tan\left(\phi_l + l\pi/2\right)\tan\delta_l\left(m_l^2 - 1\right)}{\tan\delta_l\left(1 - m_l^2\right) + \tan\left(\phi_l + l\pi/2\right)\left(1 - m_l^2\tan^2\delta_l\right)}$$

$$\left.\begin{aligned} m_l &= m_l\left(E,\alpha\right) \\ \delta_l &= \delta_l\left(E,\alpha\right) \end{aligned}\right\}\text{determined from analytical properties of Mathieu functions (tabulated)}$$

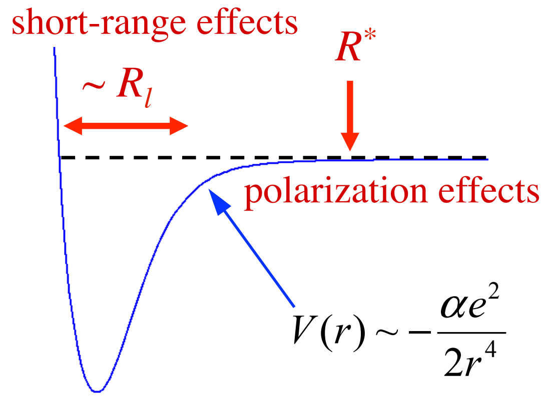
Z. Idziaszek and G. Karwasz, Phys. Rev. A 73, 064701 (2006)

K. Fedus et al., Phys. Rev A 88, 012704 (2013)

Short-range contribution:

$$\tan\left(\phi_l + l\pi/2\right) \approx B_l + R_l R^* k^2/2 + \ldots$$

the effective range expansions

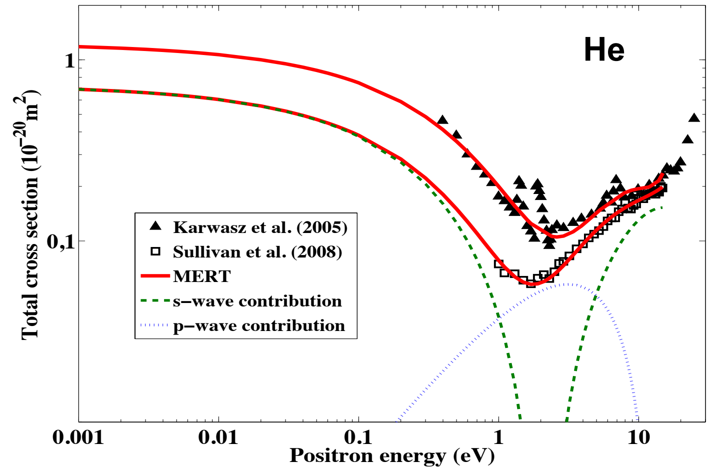


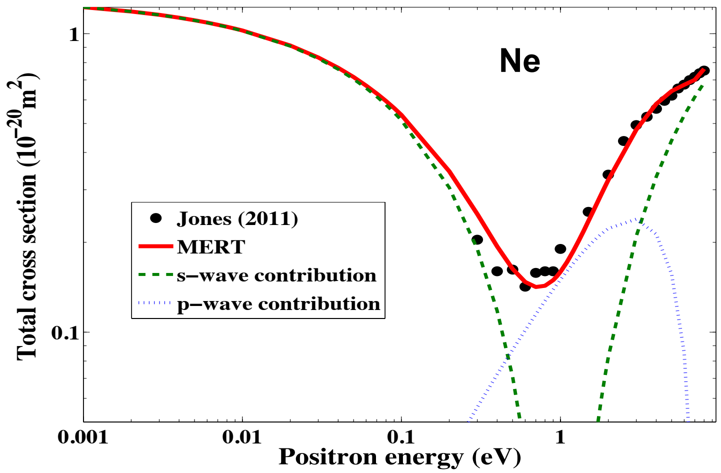
B_l – the zero energy contribution of short-range effects

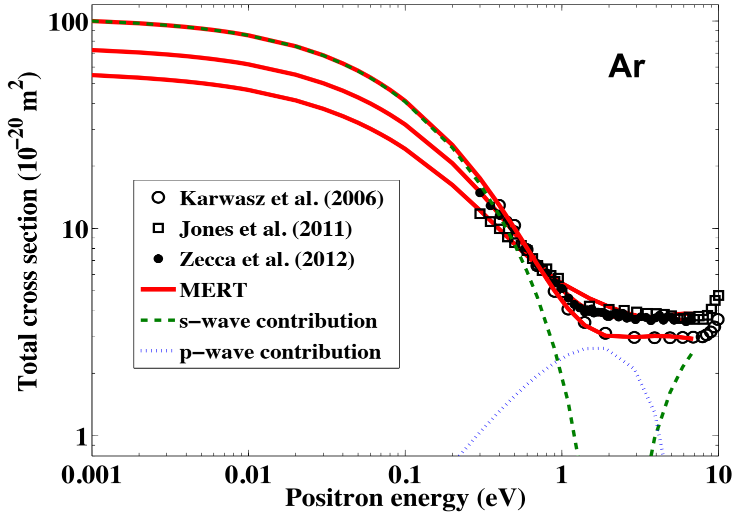
R_l – the effective range of short-range effects

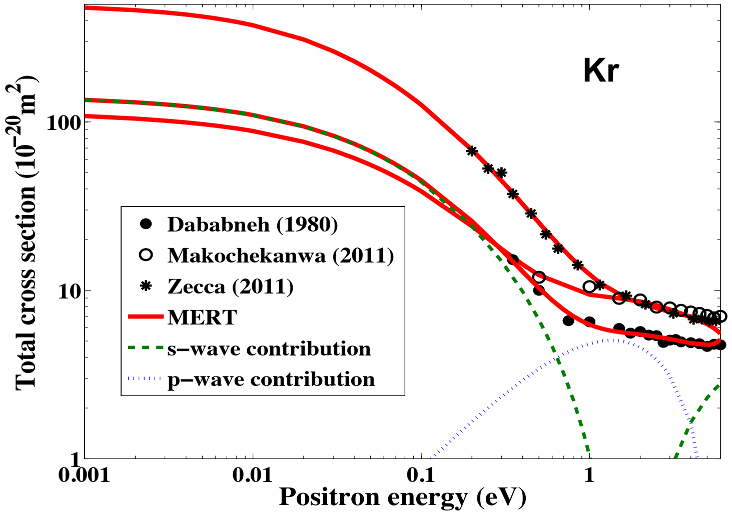
Extrapolation of total cross-section down to thermal energies by Modified Effective Range Theory (MERT)

$$\sigma(k) = \frac{4\pi}{k^2}\sum_l (2l+1)\sin^2\eta_l(k)$$



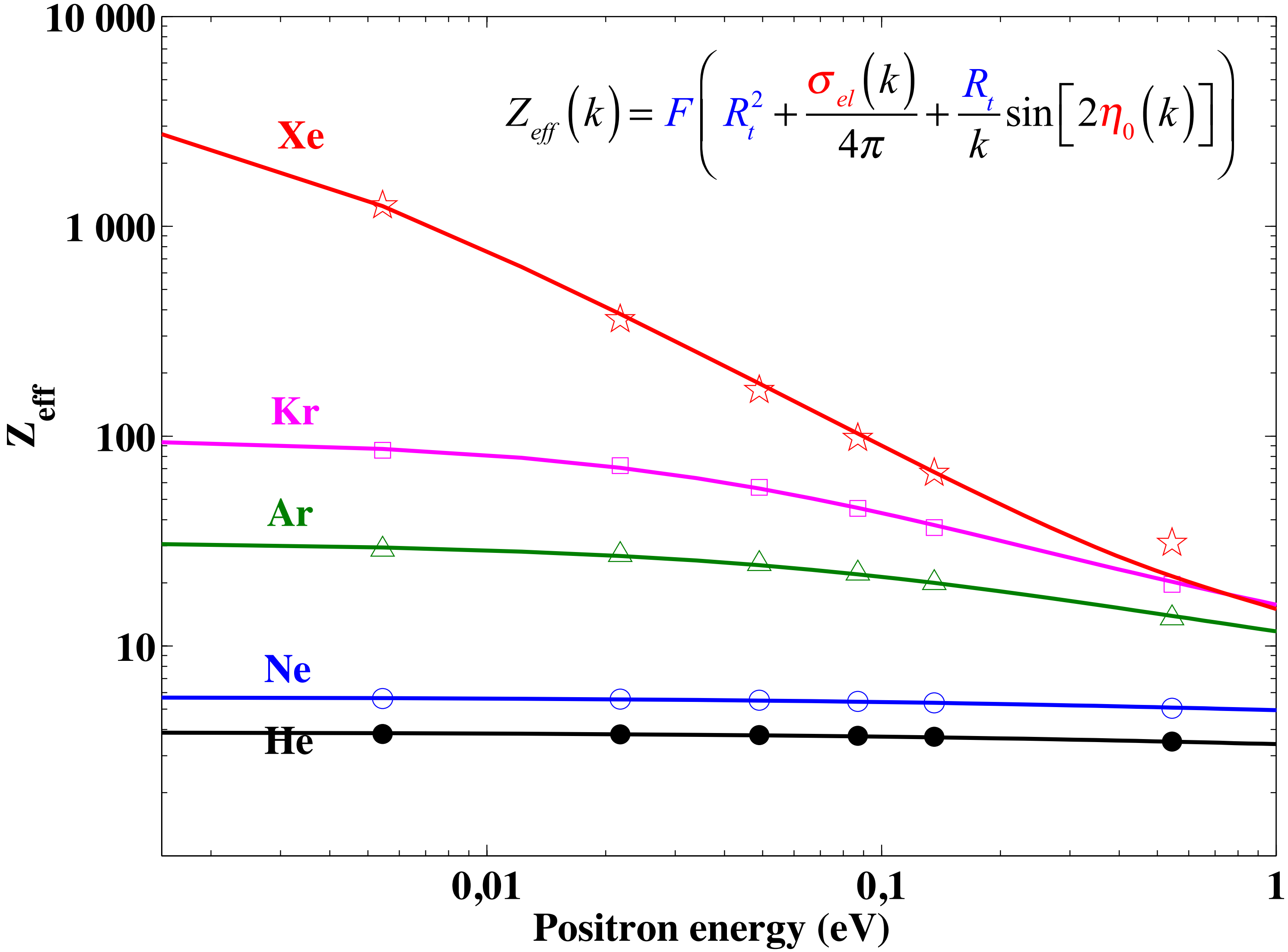






K. Fedus, G. Karwasz, Z. Idziaszek, Phys. Rev. A. 88, 012704 (2013)

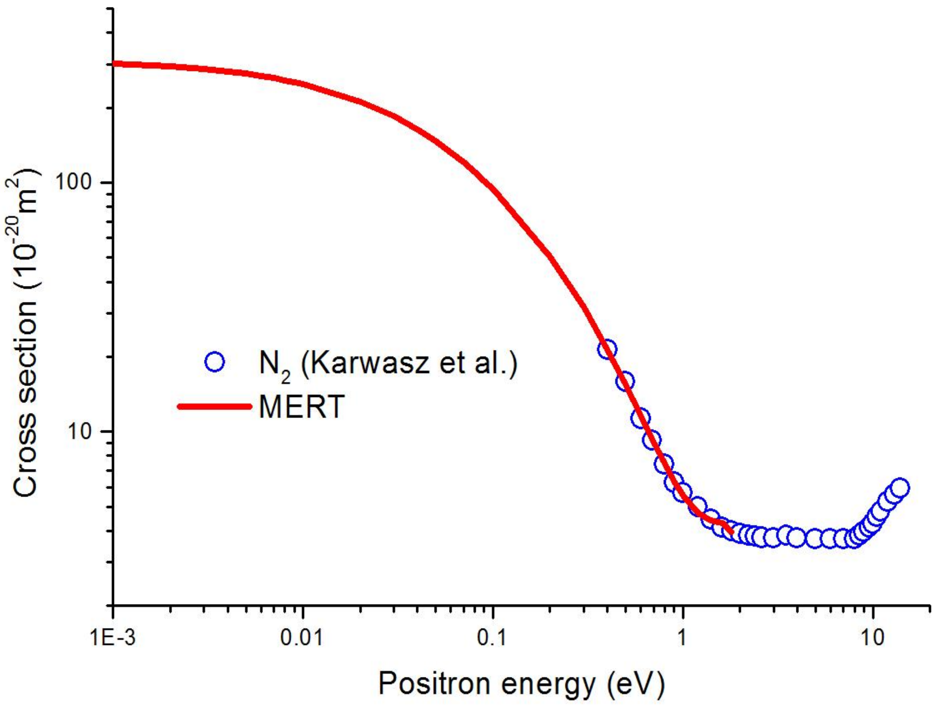
Fit to Z_{eff} data

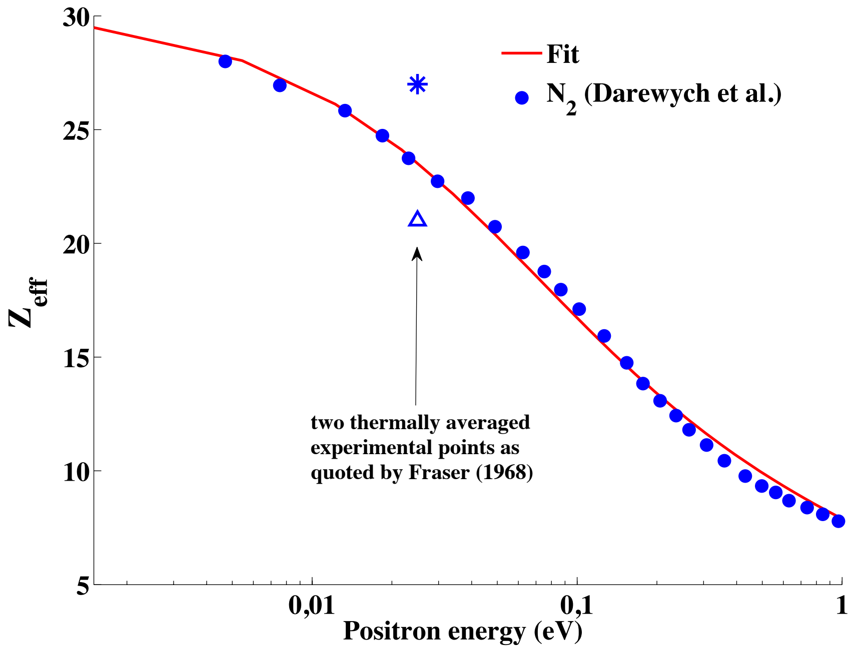


Z_{eff} from D. G. Green, J. A. Ludlow, and G. F. Gribakin, Phys. Rev. A 90, 032712 (2014)

Positron direct annihilation vs elastic scattering cross-section

Simple molecular target: N_2





G.P. Karwasz, D. Pliszka, R.S. Brusa, Nucl. Instr. Meth. B, 247, 68 (2006)

J. W. Darewych and P. Baille, J. Phys. B: Atom. Molec. Phys. 7 (1974)

P.A. Fraser, Adv. atom. molec. Phys. (New York Academic Press) 4 63-107 (1968)

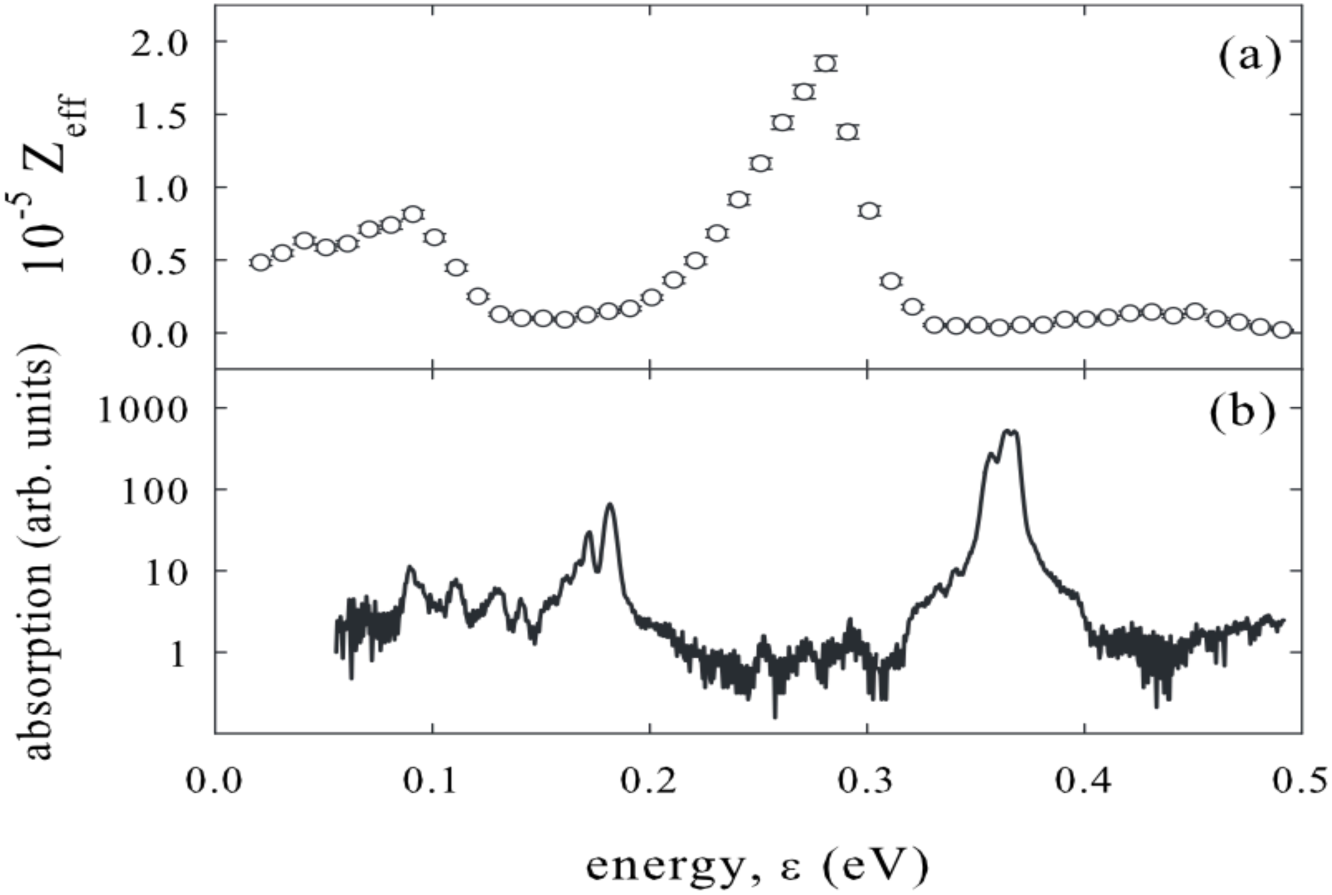


FIG. 1. (a) Z_{eff} spectrum [5]; and (b) infrared absorption spectrum (log scale, arbitrary units) [12] for hexane. Note that, when the 80 meV downshift of the Z_{eff} spectrum due to the positron-hexane binding energy is taken into account, the strong peaks in the two spectra occur at the same energy.