Data for Modeling of Positron Collisions and Transport in Gases

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Thanks to M Brunger, J Marler, C Surko, M Charlton, R Campeanu, G Garcia R. White, M Suvakov, R McEchran, C Makochekanwa, D Van Der Werf,

...
Motivation & Background

• Positrons are interesting
  – different Coulomb interactions (cf electrons)
  – different spectroscopy
  – Positronium formation
  – Experiments with antimatter

• Positrons are useful - applicable
  – biomedical science
    • PET diagnostic
    • positherapy
  – materials science
    • nanoscale probe of “open space” and defects in materials
  – Modeling of traps=production of antimatter
    • Generating antihydrogen relies on gas filled traps
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• publishable
Cross sections should be collected? Why?

- Application of data in dose adjustment
  - Semi empirical data used
  - More accurate and scientifically based predictions
  - Extension to new systems, complex systems, some specific channels for specific processes, ....
  - Average properties like energy deposition need to be revised as primary damage stems from very localized individual events

- Can cross sections be exploited?
  - CAN WE USE THE MEASURED BINARY COLLISION CROSS SECTIONS IN MODELING OF POSITRONS (THUS MAKING THEIR CROSS SECTIONS WORTHY OF COMPILATIONS)
  - Is it possible to develop swarm experiments to normalize the sets
  - Is it possible to develop benchmarks and experimental benchmarks
  - how to translate binary collision data to collisions in liquids and solids !!!!
1\textsuperscript{st} step – trap and thermalize positrons
2\textsuperscript{nd} step – measure positron molecule cross sections

- Gas filled traps
- Penning Malmberg Surko
- Crossed beam or beam /cell experiments
- Swarms

3\textsuperscript{rd} step – generate a complete set
4\textsuperscript{th} step – model application
Penning Malmberg Surko trap

- $N_2$, $H_2$, $CO$, $CO_2$, $CF_4$

CAMS experiment

New sources of data- gas filled traps
Surko Laricchia Charlton Zecca
CAMS ANU- SJ Buckman J Sullivan
How do we model ionized gases - swarms

- Number balance
- Momentum balance
- Energy balance

- Complete set of cross sections

- Individual cross sections not sufficient

- Basic tools: solutions to Boltzmann equation, Monte Carlo simulations, very accurate experiments, transport data and rate coefficients
Positron-matter interactions: Cross sections

Elastic Scattering

$e^+ \rightarrow E_o \rightarrow e^-$

Inelastic Scattering

$E_o \rightarrow E_1 < E_o$
- Electronic
- Vibrational

Ionization

Direct Annihilation

Ps Formation

Direct

511 keV
Positron-matter interactions

Elastic Scattering

\[ e^+ \rightarrow E_o \rightarrow e^- \]

Inelastic Scattering

\[ E_o \rightarrow E_1 < E_o \]

Electronic

Vibrational

Ionization

Ps Formation

Direct

Annihilation

511 keV
Inelastic Scattering

Elastic Scattering

Positron - matter interactions

E

\( E_0 \)

\( E_1 < E_0 \)

Direct Annihilation

511 keV

Ionization

Ps Formation

Direct
Ionization of Argon


6.8 eV = E_b

Cross section ($a_0^2$)

Energy (eV)

Total Ionization
Direct Ionization
Positronium Formation
Total cross sections were measured by Kauppila and coworkers [1] and total elastic cross sections were calculated by McEchran [2]: theoretical data allowed us to separate elastic and inelastic processes.

We have extrapolated the theoretical results to low and high energies.

The positronium formation and ionization were taken from Marler et al [3] while direct annihilation has been neglected.

Measured excitation cross sections for the lowest states of argon were used [4].

We have also added the cross section for higher singlet levels for electron excitation [5] of argon.
Ar total:


[a2] McEchran [personal communication].

Ps. formation and ionization


Electronic excitation:


[a5] A.V. Phelps and K. Tachibana personal communication (1985)- higher singlet states for e-Ar
HYDROGEN

a complete set of cross sections

- Total elastic cross sections were measured by Hoffman et al. [c1]
- Cross sections for electron excitations X-E and X-C were taken from Arretche and Lima [c2] and for X-B from Sullivan et al. [c3]
- The positronium formation and ionization were taken from Fromme et al. [c4]
- Vibrational cross section for v1 mode was taken from Sullivan et al. [c5] and for 0-2 and 0-3 from Gianturco and Mukherjee [c6]
- Rotational excitation the same as for electrons [c7]
$H_2$


**Electronic excitation:**  X-A and


**Ps.formation**


**Vibrational excitation**


0-2 0-3 [c6] Gianturco Mukharje

**Rotational excitation:** just like electrons?? [c7] ANU data

Feb 5, 2008
NITROGEN
a complete set of cross sections

- Total cross sections were measured by Hoffman et al. [b1] and total elastic cross sections were calculated by de Carvalho et al. [b2].
- The positronium formation and ionization were taken from Marler and Surko [b3], while direct annihilation has been neglected.
- Added the cross sections for electron excitations [b4]
- Vibrational cross sections were taken from Gianturco and Mukherjee [b5]
- Rotations Gerjoy Stein for electrons
$N_2$ total:


Ps. formation


Electronic excitation:


Vibrational excitation


Rotational excitation: Gerjoy Stein formulas- non-resonant
CF$_4$

set of cross sections

Cross sections for electronic excitations are missing! They are not available in the literature!
WATER VAPOUR
a complete set of cross sections

Total cross section

Ps formation cross section

Cross section [10^-16 cm^2]

Energy [eV]

Zecca et al.
Sueoka et al.
Beale et al.
Baluja and Jain
Gianturco et al.
Baluja et al.
De Hang et al. - modified
De Hang et al. - unmodified
Makochekanwa et al. - uncorrected
Makochekanwa et al. - corrected
Baluja et al. - normalized to CAMS at 60 eV

Makochekanwa et al.
Murtagh et al.
Harvieux et al.
our contribution to collision and transport database

electrons:

\[ \text{H}_2, \text{D}_2, \text{CO}, \text{SF}_6, \text{Ar}, \text{SiH}_4, \text{Si}_2\text{H}_6, \text{CF}_4, \text{NO}, \text{N}_2\text{O}, \text{C}_2\text{H}_2\text{F}_4, \text{HBr}, \ldots \]

ions:

\[ \text{Ne}^+, \text{F}^-, \text{Cl}^-, \text{CF}_3^-, \text{O}^-, \text{SF}_6^- \]

positrons:

\[ \text{Ar}, \text{H}_2, \text{N}_2, \text{H}_2\text{O}, \text{CF}_4 \]

transport data:

\[ \text{drift velocities, mean energies, characteristic energies, diffusion coefficients, ionization coefficients, rate coefficients, distribution functions} \]

http://mail.ipb.ac.rs/~cep/ipb-cnp/ionsweb/database.htm
Positron transport in gases:
The ultimate non-conservative transport
**Transport coefficients**

**Monte Carlo simulations**

**drift velocity**

\[ w_i = \frac{d}{dt} \langle x_i \rangle \quad \text{Bulk} \]

\[ W_F = \langle \vec{v} \rangle \quad \text{Flux} \]

**diffusion tensor**

\[ D_{Bxx} = \frac{1}{2} \frac{d}{dt} \left( \langle x^2 \rangle - \langle x \rangle^2 \right) \]

\[ D_{Fxx} = \langle xv_x \rangle - \langle x \rangle \langle v_x \rangle \]

\[ \approx w - \frac{2 \langle \epsilon \rangle}{3e} \frac{d \langle \nu_a(\epsilon) \rangle}{dE} \approx w - \frac{2 \langle \epsilon \rangle}{3e} \frac{d \nu_a(\langle \epsilon \rangle)}{d\langle \epsilon \rangle} \frac{d\langle \epsilon \rangle}{dE}. \]
Argon: a case study?!
Argon: Electrons and Positrons Mean Energies

Slightly different E/N dependence for the mean energies for electrons and positrons
Example: \((e^+, Ar)\) NDC for \(W\) (not \(w^*\))

Monte-Carlo

\[\text{Negative differential Conductivity - NDC}\]

Significantly different behavior of drift velocities for electrons and positrons!

\[\nu'_{R} > 0, \ W < w^*, \ ‘attachment’ \ cooling\]

\[W \approx \int \frac{2\langle \epsilon \rangle d\langle \nu_a(\epsilon) \rangle}{3e dE} \approx \int \frac{2\langle \epsilon \rangle d\nu_a(\langle \epsilon \rangle)}{3e d\langle \epsilon \rangle dE} \]

"R" = Ps formation
What is NDC?

NDC – decrease of the drift speed with increasing driving field

- What is the nature of the NDC?
- Electrons vs positrons
- Non-conservative processes
- What is the role of non-conservative processes?

Example – H₂ and N₂

The difference between electron and positron’s transport properties.

There is no NDC for positrons in N₂!!

The explanation is hidden in cross sections.

Shape of mean energy dependence on E/N can reveal more about cross sections!

N₂ is a better choice for buffer gas in collisional traps than H₂!
**Example – water vapour**

The shape of the mean energy reflects the energy dependence of the cross sections.

Huge difference between the flux and bulk components of the drift velocity! Strong pronounced NDC!
Was any of this observed


- Drift velocities (actually w/Zeff) measured in H₂ show NDC, and flux drift velocities do not

- MC simulation of lifetime spectra contains mobility edge:


able to that of the best available experiments. In the present work an additional energy threshold, namely the positron mobility edge $E_{c}^{+}$, is added to the FE simulation. Below $E_{c}^{+}$ the electric field is “turned off” until the positron reaches $E_{R}$ below which it forms the cluster. The mobility edge is assumed to have no effect on the form of the collision cross sections involved. The input
Drift velocity [m/s]

$e^+ - H_2$

Drift velocity [m/s] vs. $E/N$ [Td]

- Black line: positrons drift velocity - Bose, Paul, Tsai
- Red line: positrons - flux
- Green triangles: positrons - bulk
What else is there?
(Apart from the known and the unknown-Harold Pinter)

Molecular targets,

• Hydrogen Argon Nitrogen Water vapour
• $\text{CF}_4(+\text{N}_2)$

• Possibly $\text{O}_2$ CO hydrocarbons SF$_6$
• ... protein like, DNA like
Atomic Cross Sections

$e^+ - \text{He}$

Cross Sections

Gran Total
Total - Ps
Total Ps
$2^1S$
$2^1P$

Total Cross Section ($10^{-16}$ cm$^2$)

Energy (eV)

He – total scattering

$e^+ - \text{He}$

Total Cross Section

Total Cross Section ($10^{-16} \text{ cm}^2$)

Energy (eV)

Mizogawa et al.
Wu et al.
Ludlow & Gribakin
Van Reeth & Humberston
Present data

He – electronic excitation

Caradonna et al.  
PRA, 2009

Theory  
Utamuratov et al.  
2009
Total Scattering Ne, Ar, Kr, Xe

Ps Formation Ne, Ar, Kr, Xe

Ps – H$_2$
Available data:
• Ps formation
• direct and total ionization
• $A^1\Pi$ electronic excitation
• vibration $v1$
• total cross section (theoretical 10-5000 eV)
• differential for elastic (+ vib + rot)

Missing data:
other electronic and vibrational excitations

FIG. 6. Integral cross sections for CO: (●) positronium formation, (▼) direct ionization, and (◼) total ionization.
Marler & Surko, PRA 72 (2005) 062713

FIG. 13. Integral cross sections for the excitation of the $A^1\Pi$ state in CO by (●) positron and (square) electron impact [28]. Also

v1 vibrational mode of CO. Sullivan, Gilbert & Surko, PRL 86 (2001) 1494
O₂

Available data:
• Ps formation
• direct and total ionization
• vibration v1
• total cross section (experimental measurements at low energies and theoretical calculations in the range 10-5000 eV)
• differential for elastic (+ vib + rot)

Missing data:
• electronic excitations
• vibrational excitations
• rotational excitations
Available data:
- Ps formation
- direct and total ionization
- vibration v2 and v3
- total cross section
- differential for elastic (+ vib + rot)

Missing data:
- vibration v1
- electronic excitations

**CO$_2$**

Gianturco & Paioletti, PRA 55 (1997) 3491

Hoffman et al., PRA 25 (1982) 1393
$\text{SF}_6$

Important in applications of rotating wall technique.

The only available data in literature is on total cross section!

Missing data:
- $\text{Ps}$ formation
- direct and total ionization
- electronic excitations
- vibrational excitations
- differential cross sections

CHOOH (formic acid)

CAMS measurements:

**Figure 6.** Present positron impact HCOOH GTCS, GTCS – $Q_{Ps}$ and $Q_{Ps}$ compared with literature for GTCS and elastic integral (ECS) results (a) over the whole energy range of measurement and (b) below 30 eV.

**Figure 7.** Present positron impact HCOOH GTCS, GTCS – $Q_{Ps}$ and $Q_{Ps}$ results in the vicinity of the Ps threshold ($E_{Ps} = 4.53$ eV).

Ps – “Bio Molecules”

- Water: 10 electrons
- Formic Acid: 25 electrons
- THF: 40 electrons
- Pyrimidine: 42 electrons
- 3h-THF: 47 electrons
- Uracil: 58 electrons
Ps – importance of structure

Ps Formation Cross Section ($A^2$)

Energy (eV)

- He
- Ne
- Ar
- Kr
- Xe
- H$_2$O
- HCOOH
- C$_2$H$_6$O
- C$_2$H$_2$N$_2$
- C$_2$H$_4$O$_2$
- C$_2$H$_5$N$_2$O$_2$
Application of data to model a Surko trap
Standard Surko trap

![Graphs showing potential, distribution, mean energy, and radius over time for a Surko trap system.](image)
Standard Surko trap
Rotating wall +
Penning Malmberg Surko trap

- $\text{N}_2$, $\text{H}_2$, $\text{CO}$, $\text{CO}_2$, $\text{CF}_4$

Rotating wall

Particle motion without collisions

Collisions necessary
Gradient necessary
Rotating wall

![Graph showing time vs. normalized mean radius and normalized mean energy](image)
Can we apply (sell) elementary AM-positron data for modelling of medical procedures (NIH)?

• we got water balloon model- water cross sections- tracks -transport coefficients etc.

4th step: application of atomic data and models of ionized gases for PET and positron therapy
Medicine: science about human beings and how to repair them

- What is a man/woman: a water (bag) balloon - in a tradition of a spherical cow

Dense gaseous medium - transport
Tracks in human body I.E. water
Positron/secondary electron trajectories in water vapour

- e+ inelastic collisions
- e+ elastic collisions
- e+ ionization
- e+ Ps formation
- trajectory
- e- collisions
In most of those examples atomic and molecular processes served as Maxwell’s demon in controlling the EEDF and spatial profiles. In Gaseous electronics/positronics some molecular processes as described by their cross sections may play the role of Maxwell’s demon.
Conclusions

- New advances in measurements of the positron scattering data enable simulations,

- Swarm experiment would not be an efficient trap but it is experiment testing the limits of the present day techniques in kinetic theory for reactive gases

- A swarm experiment would provide means to normalize cross section sets. Positron swarms is a new frontier with new kinetic effects due to the non-conservative nature of the transport.

- Water vapour- positron interactions are well represented

- Important medical applications

- Efficient models of gas filled traps and possible optimization!!!

- Physical explanation of the rotating wall in single particle regime

- NOW IS THE RIGHT MOMENT TO SET UP A POSITRON MOLECULE SCATTERING DATA BASE