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TSAPS Fall 2003

Results for Positron-Acetylene Scattering
Using the Distributed Positron Model

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and
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Special thanks to Mr. Lee Burnside for cluster construction and maintenance.
Abstract for TSAPS 2003

Results for Positron-Acetylene Scattering Using the Distributed Positron Model,
THOMAS L. GIBSON, Texas Tech University, and PATRICK J. NICHOLS, University of New
Orleans — The Distributed Positron Model (DPM) has been developed as a means to include the
correlation/polarization interaction between a slow positron and an atomic or molecular target.
This technique is based on a quantum chemistry approach that approximates the effect of virtual
positronium formation near the target and automatically reduces to the correct long-range form of
the polarization potential far from the target. Further, the codes that implement our DPM
method have been written to run on low-cost concurrent computers known as GNU/Linux Beowulf
clusters. In this talk we will report integrated and differential cross sections for low-energy
positron-acetylene collisions.
Motivation

Why calculate low-energy positron-molecule collisions?

- Very few measured results available
  - Intense low-energy beams are hard to achieve
- Existing experiments don’t agree
- Most theories too parameterized or intractable for larger systems
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Integrated Cross Sections

Dababneh et al (1988)
Sueoka and Mohn (1986)
Charlton et al (1983)

\( ^{12} \text{CH}^4 \rightarrow \ ^{14} \text{CH}^4 \)

Energy (eV)

Cross Section (Å²)
Energy (eV) vs. Cross Section (10^{-16} cm^2)

- Hoffman et al. (1982)
- Charlton et al. (1983)
- Sueoka and Mori (1984)

Integrals of Cross Sections
Energy (eV)

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

Charlton et al (1983)
Sueoka and Mori (1984)

Integrated Cross Sections

TTU
TTU

D - Å

BE

0246810

Energy (eV)

Energy (eV)

Cross Section (Å²)


Sueoka et al (1997)

Integrated Cross Section

\( \text{e}^+\text{SF}_6 \)

\( \text{SF}_6 \rightarrow \text{SF}_6^- \)
Our Theoretical Treatment

- Isolated collision between one target (atom or molecule) and one positron of known kinetic energy
- Only elastic scattering—stay below the energy threshold for electronic excitation of the target or for real positronium formation
- Local, energy-independent interaction potential based on physically-motivated approximations
Reduction of Scattering Formulation

We “reduce” the problem by expanding the (N+1)-particle ket in a complete set of target and scattering states, viz.

$$|\Psi> = \sum_\gamma F_\gamma \Phi_\gamma.$$ 

Using this expansion in the T.I.S.E. and operating on the left with $< \Phi_0|$ eventually leaves the one-particle T.I.S.E. for elastic scattering of the positron

$$\hat{T}_p |F_0> - \frac{k^2}{2} |F_0> = -\hat{V}_{sp} |F_0> .$$
Interaction Potential

A local approximation to the interaction potential between a colliding positron and the molecular target can be represented as

\[ V_{sp}(\vec{r}_p) = V_{st}(\vec{r}_p) + V_{pol}(\vec{r}_p), \]

where the static potential is given by,

\[ V_{st}(\vec{r}_p) = \langle \Phi_0(\vec{r}_i) | \hat{V}_{int} | \Phi_0(\vec{r}_i) \rangle, \]

with \( \hat{V}_{int} \) representing the Coulomb interactions between the positron and the target and where \( V_{pol}(\vec{r}_p) \) is the polarization potential.
Polarization Potential

The polarization potential is defined as the energy difference

\[ V_{pol}(\vec{r}_p) = E^R(\vec{r}_p) - E^U(\vec{r}_p), \]

where the energy from the relaxed (distorted) target orbitals is

\[ E^R(\vec{r}_p) = \langle \Phi^R(\vec{r}_i; \vec{r}_p) | \hat{H}_t + \hat{V}_{int} | \Phi^R(\vec{r}_i; \vec{r}_p) \rangle_{d\vec{r}_i}, \]

and the energy from the unrelaxed (ground state) orbitals is

\[ E^U(\vec{r}_p) = \langle \Phi^U_0(\vec{r}_i) | \hat{H}_t + \hat{V}_{int} | \Phi^U_0(\vec{r}_i) \rangle_{d\vec{r}_i}. \]

In the adiabatic approximation, both \( E^U(\vec{r}_p) \) and \( E^R(\vec{r}_p) \) are calculated by treating the projectile as an additional “proton” (located at \( \vec{r}_p \)) and using an LCAO:MO SCF Quantum Chemistry code to provide variational estimates of these energies.
Nuclear Attraction Integrals

The distortion of the molecular orbitals is driven by the nuclear attraction integrals that involve the positron as an additional “nucleus” at $\vec{r}_p$.

$$I_{i,j}^{N_{AI}} = \langle \alpha_i(\vec{r}_e) | V(\vec{r}_e; \rho_{pos}) | \beta_j(\vec{r}_e) \rangle,$$

where the interaction $V$ from a distribution of positive charge $\rho_{pos}$ is given as

$$V(\vec{r}_e; \rho_{pos}) = \int d\vec{r} \rho_{pos}(\vec{r}) \frac{-1}{|\vec{r}_e - \vec{r}|}.$$

For the adiabatic approximation, $\rho_{pos}(\vec{r}) = \delta(\vec{r} - \vec{r}_p)$, which is appropriate for the positive charge distribution in a virtual H atom.

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Virtual Positronium vs Virtual Hydrogen

- Adiabatic approximation is much too attractive in the near-target region
- Use $\rho_{pos}$ more nearly correct for virtual Ps
  - Hence, the name Distributed Positron Approximation (DPM)
Figure 1: Unlike the H atom, the positive charge in the Ps atom is not localized at the C.O.M. of the atom.
The Distributed Positron Model

We have investigated several simple choices of $\rho_{pos}$ that reflect the distribution of positive charge in a Ps atom and lead to a polarization potential that reduces to the correct long-range behavior of the polarization potential, including:

- Uniform Spherical
  - $R_p = 1.5$ Bohr (Average radius of Ps atom)
  - $R_p = 1.0$ Bohr (Maximum radial probability of Ps atom)
- H1S distribution
- STO-3G distribution
For specificity, consider the following case:

- Diatomic target with nuclei at \( \vec{A} \) and \( \vec{B} \)
- Additional “nucleus” (positron) with charge distribution \( \rho_{pos} \) located at \( \vec{C} \equiv \vec{r}_p \)

**Figure 2:** A distribution of positive charge simulates the effect of virtual Ps formation in the DPM.

[Image of the diagram with labels for \( \vec{A} \), \( \vec{B} \), \( \vec{C} \), \( e^- \), \( r_c \), \( e^+ \)]
The DPM Distortion Interactions $s_{odd} \Delta V_{\rho_{\text{pos}}}^{(r)}$ for various choices of $\rho_{\text{pos}}$ in $\rho_c$. The DPM Distortion Interactions.

Figure 3: The distortion interaction $\Delta V_{\rho_{\text{pos}}}^{(r)}$ for various choices of $\rho_{\text{pos}}$ in $\rho_c$. The DPM Distortion Interactions.

![Graph showing DPM Distortion Interactions](image)
Computing the Interaction Potential

To calculate the polarization component of the interaction potential, we fix the positron at a large number of points near the target and then compute a variational estimate of the system energy for each of these points.

- **Bigger Systems ⇒ More CPU Time**
  - Time to compute $V_{pol}$ for Ar: 12 minutes (serial code)
  - Time to compute $V_{pol}$ for SF$_6$: 125 days (estimated)

- **Bigger Systems ⇒ More Memory**

- **Bigger Systems ⇒ More I/O**
Solution

- **Beowulf Cluster**
  - Performance: 100’s to 1000’s of Megaflops
  - Memory: Gigabytes
  - I/O: Distributed Across Multiple Nodes
  - **Very** Affordable Hardware
  - Standard Software Available for Free
  - Local Control
    * Configuration Optimized for Problem
    * No Sharing Required
**Gamera Mark II Hardware**

- 32 1-GHz Athlon CPUs
- 16 Gigabytes aggregate ram
- 640 Gigabytes aggregate disk
- 2 100 base-T 24-port switches
- **Cost** $\sim 30,000
Positron-$\text{C}_2\text{H}_2$ Polarization Potential

Distance from COM (Bohr)

Polarization Potential (Hartree)

- transverse axis polarization
- parallel axis polarization
Positron-C$_2$H$_2$ Integrated Cross Sections

![Graph showing integrated cross sections as a function of energy (eV). The graph compares data from Sueoka et al. and DPM models. The data points for Sueoka et al. are represented by squares with error bars, while the DPM model is represented by a continuous blue line.](http://www.phys.ttu.edu/~ritlg/)
Positron-C$_2$H$_2$ Differential Cross Sections

![Graph showing DCS (a$_0^2$ sr$^{-1}$) vs. Scattering Angle (degrees) for different energies (0.5 eV, 1.0 eV, 2.0 eV, 3.0 eV, 4.0 eV).]
Conclusions

- High-Performance Computing ≡ Concurrent Computing
- Affordable Parallel Systems Are Available Now
- Open Source Software and Scientific Applications Are Compatible
- The DPM has been shown to yield consistently good agreement with measured low-energy positron-atom and positron-molecule collisions

We are grateful for the collaborative efforts of Dr. Robert Lucchese and Dr. Franco Gianturco on the CH₄ and SF₆ systems, as well as our continuing work on C₈H₈.
Integral Cross Sections

Integration Cross Sections

Energy (eV)

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

Charlton et al (1983)
Sueoka and Mori (1984)
DPM (STO-3G)
DPM (US Rp=1.5)

http://www.phys.ttu.edu/~ritlg/
Energy (eV) vs. Cross Section (10^{-16} cm^2)

Charlton et al (1983)
Sueoka and Mori (1984)
DPM (STO-3G)
PCOP (Density Functional)

Integrated Cross Sections

Position CO_2 Cross Sections
TTU

Energy (eV)

Cross Section (Å²)

Integrated Cross Section

\[ e + SF_6 \]

Dababneh et al (1988)
Sueoka et al (1997)

Integrated Cross Section

Position-SF\textsubscript{6} Cross Sections - Close
**C$_2$H$_2$ Properties - 1**

Table 1: Total Energies

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<tr>
<th>Research Group</th>
<th>Energy (Hartree)</th>
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<tr>
<td>this work</td>
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<td>Jameson and Fowler</td>
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<td>Lindh and Liu</td>
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## $\text{C}_2\text{H}_2$ Properties - 2

**Table 2: Quadrupole Moments**

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<td>experimental</td>
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Table 3: Polarizabilities

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