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Friedrich Aumayr
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Institut für Allgemeine Physik
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ATOMIC AND MOLECULAR PHYSICS USING POSITRONS IN A PENNING TRAP

C. M. Surko,[a] Koji Iwata, R. G. Greaves, C. Kurz, and S. J. Gilbert
Physics Department, University of California, San Diego,
La Jolla, California, 92093-0319, USA

We have developed methods to accumulate and cool large numbers of positrons in a Penning-Malmberg trap. These collections of room-temperature positrons provide a powerful tool for studies of atomic and molecular physics. Recent research in this area is summarized, including the development of a method to create an ultra-cold positron beam, measurement of inner-shell annihilation in noble gases, and the localization of annihilation sites in hydrocarbon and fluorocarbon molecules.

1 Introduction

The interaction of atoms and molecules with low-energy positrons has been studied since positron sources became widely available in the 1950's.[1] The experimental techniques for such studies have advanced considerably since then.[2] In the last decade, the development of Penning-Malmberg traps to efficiently accumulate positrons[3] has provided new opportunities to study positron-atom scattering and annihilation processes.[4,5,6,7,8,9] In this paper, we describe recent technological developments and briefly review several new measurements in this area.

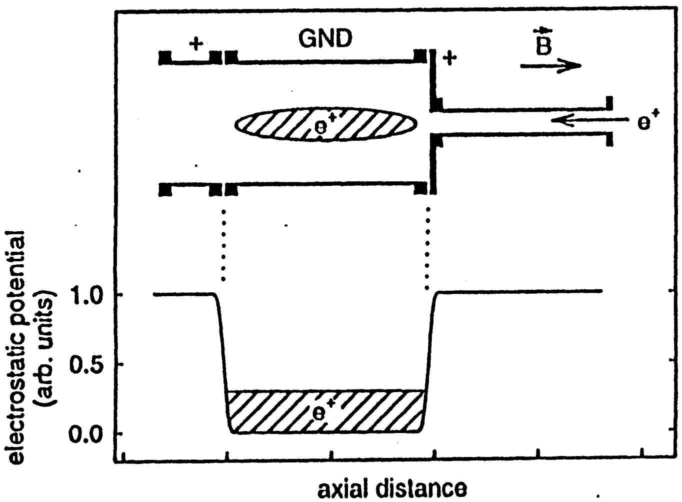
2 Experimental arrangement

2.1 Positron trap

The Penning-Malmberg trap was originally developed to achieve long-time confinement of electrons.[10] This technique has also proven to be advantageous for trapping antiparticles such as positrons and antiprotons. Surko *et al.* modified this technique to efficiently accumulate large numbers of positrons.[3] Figure 1 shows the last stage of the three-stage positron trap they developed. Radial confinement is provided by an applied magnetic field, and axial confinement is provided by potentials on a set of electrodes.

Positrons with energies up to 540 keV are obtained from a 35-mCi ^{22}Na source. They are moderated (i.e., slowed) to a few eV by a solid Ne film. The resulting low energy positrons (~ 30 eV) are injected into the trap, where they

[a] Invited speaker and corresponding author: csurko@ucsd.edu.



igure 1: Schematic diagram of the positron trap. The electrode structure of the final stage [the three-stage positron trap is shown (above). The corresponding electrostatic potential for positron confinement is also shown (below).

Table 1: Positron trap performance.

Source strength	Incident slow positron flux	Trapping efficiency	Maximum positrons trapped	Positron lifetime
35 mCi	3×10^6 e^+/s	30%	1×10^8 in 3 min	2 hr

.re confined and cooled by inelastic collisions with a buffer gas of nitrogen nolecules. Details of the trapping mechanism are discussed elsewhere.[11]

The performance of the trap is summarized in Table 1. With the nitrogen ›uffer gas in the trap, the lifetime of positrons is limited by annihilation on the ;as. The nitrogen gas can be pumped out in the order of 8 s following positron oading. In the resulting ultra high vacuum (UHV) environment ($\sim 5 \times 10^{-10}$ Corr), the positron lifetime is about two hours, limited by annihilation on npurities in the system.

2.2 *An ultra-cold positron beam*

Positron beams with narrow energy spreads have many potential applications, including studies of atomic and molecular physics. Examples include a variety

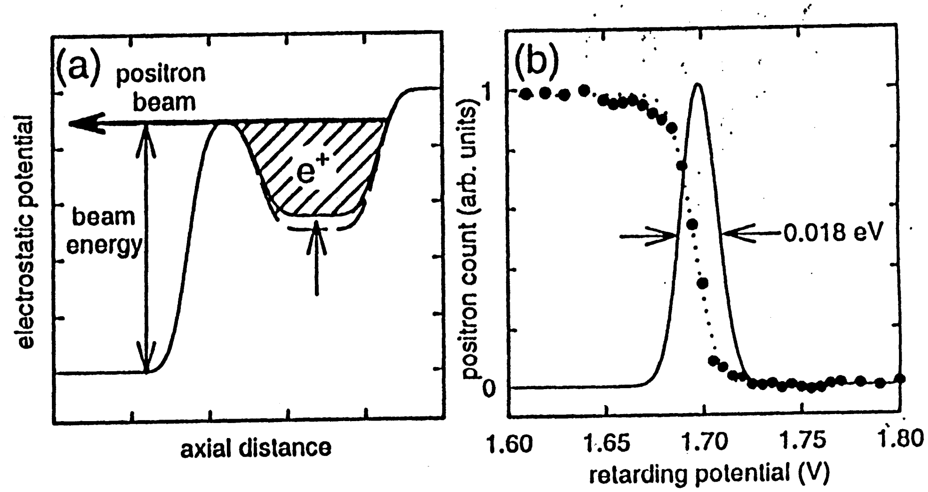


Figure 2: The creation of an ultra-cold positron beam. (a) Arrangement of potentials in the third stage of the trap. The positrons cool to room temperature, and then the potential is raised slowly until the positrons spill out of the trap. (b) Axial energy distribution of the resulting positron beam: (•) observed positron counts, (···) fit to the data, and (—) axial energy distribution.

of resonance-type behavior in the interaction of positrons with atoms, such as a resonance in the annihilation rate recently predicted to occur just below the positronium formation threshold energy.[12,13] Another example is the production of unfragmented molecular ions by positronium formation in a narrow range of energies above the threshold.[14]

Recently, we have been able to create a positron beam with a very narrow energy spread using the positron trap as a source for the beam.[15] A schematic diagram of this technique is shown in Fig. 2(a). The stored positrons are allowed to spill over the trapping potential by raising the bottom of the potential well, as indicated by the upward arrow in the figure. The energy of the beam can be tuned by adjusting the potential of the exit gate. The parallel component of positron energy is shown in Fig. 2(b) and corresponds to an energy spread of 0.018 eV FWHM.

3 Atomic and molecular physics studies

In the last decade, positron annihilation on atoms and molecules has been studied for a wide range of substances in the positron trap described here.[4,5,6,7,8,9] The positrons are typically at room temperature, and all of the experiments are done at energies below the threshold for positronium atom formation. We have concentrated on two types of measurements. The first is the measurement of annihilation rates of positrons on atoms and molecules.[7] The annihilation rate is generally expressed in terms of the normalized annihilation rate, Z_{eff}. For a small atom or an inorganic molecule, Z_{eff} is of the order of the number of electrons in the molecule, and the Z_{eff} parameter can be considered to be the effective number of electrons contributing to positron annihilation. However, annihilation rates for large organic molecules are many orders of magnitude larger than those expected from the number of electrons in these molecules.[4] The physical process responsible for these anomalously high annihilation rates is not yet understood. For atoms and single-bonded molecules, Murphy and Surko discovered an empirical scaling of annihilation rates, $\ln(Z_{eff}) = A(E_i - E_{Ps})^{-1} + B$, where A and B are constants, E_i is the ionization energy of the substance, and E_{Ps} is the binding energy of a positronium atom (6.8 eV).[5] This scaling indicates that the electronic structure of the substance is an important parameter in determining Z_{eff}. The appearance of E_{Ps} in the scaling suggests a model in which a positronium atom is loosely bound to a positive ion.

The second type of experiment is measurement of 511-keV annihilation γ-ray line resulting from the interaction of low energy positrons with atoms and molecules.[8] This line is Doppler broadened due to the momenta of the annihilating electron-positron pairs. For room-temperature positrons, this broadening is dominated by the momenta of the bound electrons. Thus, measurement of the γ-ray spectra provides information on the quantum states of the annihilated electrons.

We now have extensive data for Z_{eff} and γ-ray spectra for a wide variety of chemical species. Detailed discussions of these measurements are published elsewhere.[7,8] We would like to encourage improved calculations of these quantities to compare with the data that are now available. Below, we briefly discuss a few examples of recent measurements in this area.

3.1 Noble gas atoms

Noble gas atoms are relatively simple systems, and theoretical calculations are possible in a variety of approximations. A recent example of excellent agreement between theory and experiment is the γ-ray spectrum for He.[16] Figure 3 shows the experimentally observed γ-ray annihilation spectrum from low pressure He in the positron trap, with the Compton scattering and background components subtracted.[16] This spectrum contains the detector response, which is well approximated by a Gaussian with a FWHM of 1.16 keV. Shown by the

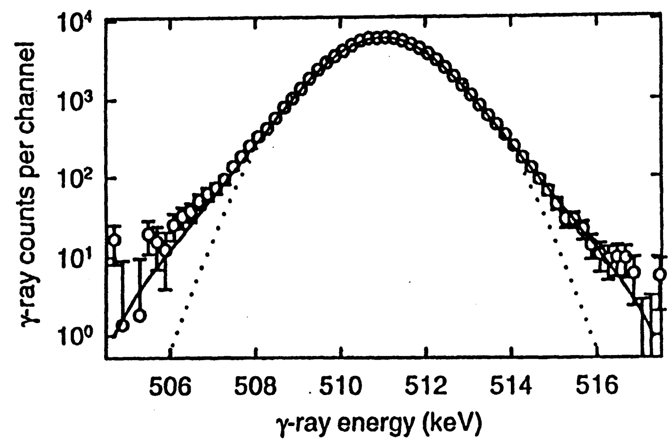


Figure 3: Positron annihilation γ-ray spectrum from He.[16] (o) experiment, (—) theoretical calculation convolved with the detector response, and (···) Gaussian fit.

solid line in Fig. 3 is a recent theoretical prediction of the spectrum calculated using the Kohn variational approximation with very accurate wave functions.[16]

The agreement between theory and experiment is excellent, extending over three orders of magnitude in spectral amplitude. In previous experiments,[17] the annihilation lines were analyzed assuming Gaussian line shapes. However, there is no theoretical reason to assume such a line shape, and our data show clear deviations from a Gaussian (dotted line).

In comparison with He, the understanding of positron annihilation on larger noble gases is less advanced. For example, there have not been any theoretical models that can explain the high annihilation rate measured for Xe.[18,19] The momentum distributions of annihilating pairs for noble gas atoms (which are equivalent to the γ-ray spectra) were calculated in the 1970's by McEachran *et al.*[20] While the resulting spectra do not agree with our observations,[8] the predicted changes of annihilation rates with positron temperature are in excellent agreement with our recent measurements[22] as we discuss below.

The positron-nucleus potential is repulsive, so that positrons cannot penetrate deeply into the electron cloud, and annihilation is found to be predominantly from the valence electrons.[8] However, a small fraction of positrons can tunnel through this repulsive potential and annihilate with inner-shell electrons, leading to a broad component in the spectra. We have investigated this effect in the noble gases, and these experiments are the first observation of positrons annihilating with inner-shell electrons in gaseous media. A detailed

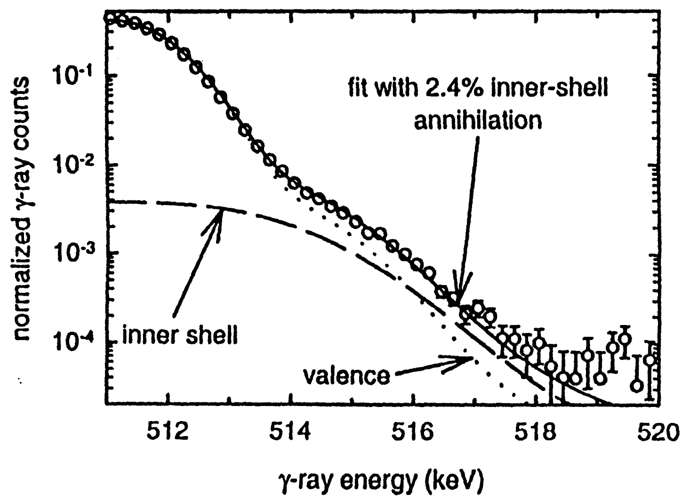


Figure 4: Positron annihilation γ-ray spectrum from Xe: (o) experiment, (—) fit using a theoretically calculated spectra with 2.4% inner-shell component, (···) valence electron component, and (- - -) inner-shell electron component.

description of these experiments is published elsewhere.[9]

The γ-ray spectrum for Xe is displayed in Fig. 4, where only the high-energy side of (symmetrical) spectrum is shown. Annihilation γ-ray spectra from each subshell were calculated using the static Hartree-Fock approximation.[9] Comparing the experimental spectrum with the calculation, the observed broad component cannot be explained by the valence electrons alone. The observed spectrum was fitted by adjusting the amplitude of the calculated inner-shell spectrum relative to that of the valence electron component. This fit indicates that 2.4% of the positrons annihilate with inner-shell electrons in Xe. Similar analyses for other noble gases indicate 1.3% inner-shell annihilation in Kr and less than 0.2% in Ar. We note that Xe and Kr have 18 electrons in the first inner shell as compared to 8 for Ar. Part of the smaller inner-shell annihilation for Ar is due to this effect.

Recently, we developed a technique for heating the positron gas confined in our trap by applying RF noise to one of the electrodes.[21] Using this technique, we were able to make the first systematic measurements of the dependence of annihilation rates on positron temperature for noble gas atoms.[22] The measured values of Z_{eff} are plotted in Fig. 5, where the data are normalized to the room-temperature values. The theoretically calculated temperature dependences (based on the polarized orbital approximation,[20] except for He[16]) are also shown in the figure. These predictions are in excellent agreement with experiment. This agreement is somewhat surprising, since the predicted absolute values of Z_{eff} at room temperature do not agree well with the measurements.[7,19]

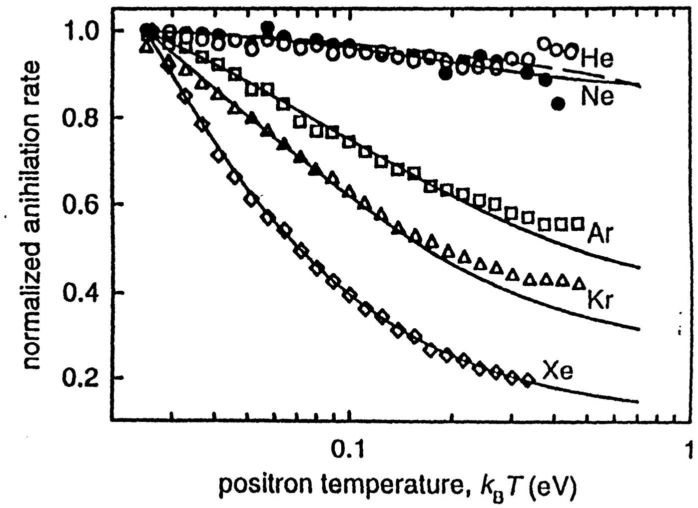


Figure 5: Temperature dependence of positron annihilation rates on noble gases. Experimental data: (•) He, (o) Ne, (□) Ar, (△) Kr, and (◇) Xe. Also shown are theoretical calculations: (- - -) Kohn variational approximation for He,[16] and (—) polarized orbital approximation.[20]

3.2 Molecules

We have now made annihilation rate and γ-ray spectral measurements for a wide range of molecules.[7,8]. To date, however, there has been much less theoretical work with the exception of a few of the simplest molecules.[23] For more complicated molecules, a semi-empirical method has been attempted.[24] Recently, large-scale calculations using the Schwinger multichannel method have begun to provide insight into the anomalously high annihilation rates observed for hydrocarbons.[25]

Our recent measurements on alkanes and partially fluorinated hydrocarbons indicate that positrons annihilate with equal probability on any of the valence electrons.[8] This is illustrated in Fig. 6. In panel (a), the observed line widths of the γ-ray spectra from alkanes are plotted against the number of valence electrons in C-C bonds. Chuang and Hogg calculated the momentum distributions of C-H and C-C bond electrons,[26] and these momentum distribu-

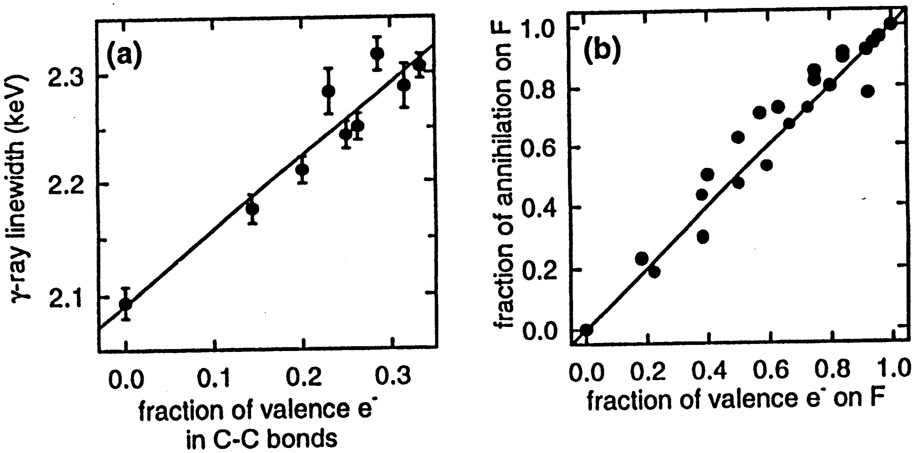


Figure 6: Studies of annihilation on valence electrons in molecules. (a) (•) observed γ-ray line width for alkanes plotted against the fraction of valence electrons in C-C bonds, and (—) fit to the data. (b) (•) Fraction of annihilation on fluorine atoms for partially fluorinated hydrocarbons plotted against the fraction of valence electrons on fluorine atoms, and (—) the line $y = x$. The linear relationship in both figures provides evidence that positrons annihilate with equal probability on any valence electron.

tions result in different characteristic line widths. Based on this calculation, the linear relationship observed in Fig. 6(a) provides evidence that positrons annihilate with equal probability on any valence electron in alkane molecules.

We have also studied this effect in partially fluorinated hydrocarbons.[8] Hydrocarbon molecules have relatively narrow γ-ray lines compared to perfluorinated carbon molecules. The measured γ-ray spectra from partially fluorinated hydrocarbons can be fit accurately using a linear combination of the experimentally measured (analogous) hydrocarbon and perfluorinated carbon spectra (e.g., by fitting the C_2H_5F spectrum with the measured C_2H_6 and C_2F_6 spectra). These fits yield the fraction of annihilations on fluorine atoms. The resulting values are plotted against the fraction of valence electrons on fluorine atoms in Fig. 6(b). As in the case of the alkanes, the linear relationship in this figure indicates that positrons annihilate with equal probability with any of the valence electrons in partially fluorinated hydrocarbon molecules.

4 A new positron trap and antihydrogen

We are currently constructing a new positron trap. With carefully designed components and simplified construction, we expect to be able to accumulate

10^{10} positrons per hour in a UHV quality vacuum.[27] This can be expected to provide a new range of scientific and technological opportunities.

One application of improved traps of this type will be the production and trapping of antihydrogen atoms.[27,28] Antihydrogen offers an opportunity to test CPT (charge, parity, time reversal) invariance with unprecedented precision and eventually to be able to test the equivalence of the gravitational attraction between matter and antimatter. While antihydrogen atoms have been created recently for the first time by passing a beam of high energy antiprotons through Xe gas,[29] these antiatoms were too energetic to be used for precision experiments. The merging of trapped antiproton and positron plasmas at low temperatures should permit the formation of low energy antihydrogen atoms that can be trapped and used for precision experiments.[30]

5 Conclusion

The positron trap described here has become a powerful tool for atomic and molecular physics. In particular, studies of low-energy positron annihilation have provided unique information about the two-body interaction of positrons with isolated atoms and molecules. Ongoing refinements in these trapping techniques and new developments in their utilization are expected to continue to expand the potential applications in this area.

Acknowledgments

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