

# **Positron Collisions with Targets of Biological and Technological Relevance**

**Alessandra Souza Barbosa**

Departamento de Física, Universidade Federal do Paraná, Caixa Postal 19044,  
81531-990 Curitiba, Paraná, Brazil

Positron physics attracts great interest due to its fundamental, technological and biological applications. And since many of its applications are based on basic interactions of positrons with molecules, positron-scattering studies become a cornerstone towards understanding the underlying physics of these interactions. In recent years, thanks to the advent of better theoretical methodologies and computers to perform the simulations, theoretical positron-molecules studies have gained new breath. At the same time, experimental advances have considerably improved the data available in the literature.

However, positron scattering calculations can be a difficult task due some intrinsic problems. For example, besides the inelastic process already observed in electron-scattering, the incoming positron can capture one of the electrons of the target to form positronium (Ps). Moreover, Ps formations can be responsible for a large amount of the total cross section for positron impact energies over the positronium formation threshold. Even more troublesome, at energies below the Ps formation and electronic excitation thresholds, the agreement between the theoretical calculations and experimental data is far from good. This is mainly due to a poor description of the polarization potential for positron scattering.

In recent years, our group put a lot of effort in order to provide some reliable results for positron scattering by molecules and systems of technological and biological relevance. For example, employing the Schwinger multichannel method [1], we have performed extensive studies in order to improve the description of the polarization potential for two small non-polar molecules, allene and silane [2,3]. It is worth mentioning that the fact that for the first time a bound

state was predicted by an *ab initio* scattering calculation [2]. Our group has also been leading the efforts of the description of positron interactions with biological systems, such as the pyrimidine molecule [4] and tetrahydrofuran [5].

In this talk we will discuss some of our recent theoretical results on positron scattering by molecules of technological and/or biological relevance. Some of the target molecules include benzene and its azaderivatives, pyridine and pyrimidine, tetrahydrofuran some small nonpolar molecules.

[1] J. S. E. Germano and M. A. P. Lima, Phys. Rev. A **47**, 3976 (1993).

[2] A. S. Barbosa, S. D'A. Sanchez and M. H. F. Bettega, Phys. Rev. A **96**, 062706 (2017).

[3] A. S. Barbosa, M. H. F. Bettega, Phys. Rev. A **96**, 042715 (2017).

[4] A. S. Barbosa, D. F. Pastega, M. H. F. Bettega, J. Chem. Phys. **143**, 244316 (2015).

[5] A. S. Barbosa and M. H. F. Bettega, J. Chem. Phys. **150**, 184305 (2019).