Rovibrational positron scattering from diatomic molecules

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Positron scattering by molecules, even the simplest ones, is a difficult theoretical manybody problem, so that few applications aiming at the calculation of scattering cross sections can be found in the literature [1, 2]. Recently, we reported the elastic and rovibrational cross sections for positron scattering from Nitrogen molecule using a three-dimensional potential energy surface for the interaction of the system in the close-coupling formalism [3]. That results showed a peaked behavior in the 0 → 1 vibrational excitation cross section which could be responsible for the existence of a virtual state, and contributed to the positron energy loss of the nitrogen buffer gas.

In this work we develop semi empirical local potentials for positron scattering from molecules. The elastic and inelatstic (rotational and vibrational) cross section for positron scattering from Oxygen, Hydrogen and Nitrogen molecules are reported using the finite nuclear mass correction (FNMC) [4] to find the potential energy surface (PES) considering a the three-body interaction potential. The scattering cross section problem are solved in a close clouping (CC) aproximation as implemented in the MOLSCAT code [5]. We report the rotational and vibrational cross sections for energies from 0.05 to 10.0eV and compare with previous theoretical and experimental results. Our results shows that inclusion of the rovibrational excitation could explain, for example, the underestimated measured reported by I. Chiari et al [6] in the low energy range.

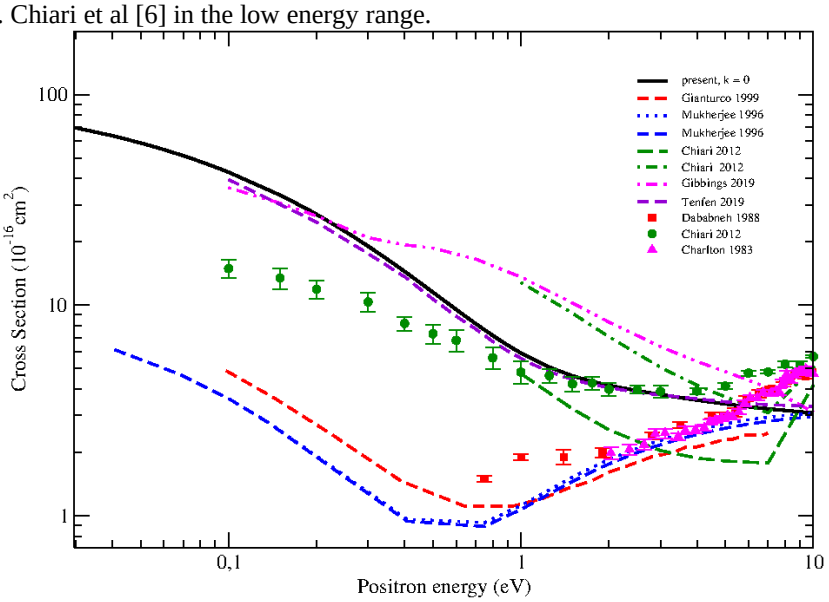

Figure 1: Total cross section for positron scattering from Oxygen molecule.

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