Modelling dynamical processes in molecular gases induced by low-energy positrons

F.A. Gianturco
Department of Chemistry, The University of Rome "La Sapienza", P.le A. Moro 5, 00185 Rome, Italy.

The availability of thermal or near-thermal positron sources have triggered in the last decade a tremendous development in the observation of processes that can occur in molecular gases once they interact with beams of these antiparticles over a broad range of low energies of chemical interest.

The processes of interest include elastic scattering, electronic and vibrational excitations, molecular ionization, positronium (Ps) formation and positron annihilation. One therefore needs to develop correspondingly articulate and flexible theoretical and computational tools that can successfully match the surprising variety of events, at the molecular level, which have been uncovered by the experiments.

In this talk I will endeavour to show a subset of examples which deal with polyatomic molecular gases and for which theory and computations have been able to provide realistic descriptions of the processes at hand. Thus, we will briefly show what can be gathered about vibrational excitation of small polyatomics (1), about the possible effects of nuclear motion on Protonation Affinities (2) and on the transient molecular deformation effects on annhilation processes (3).

I shall also try to show how one may carry out numerical "experiments" on hollow cages like C60, C20 or Cubane in order to assess the likelihood of trapping positrons inside such molecular cavities for realistic time periods (4,5), as has been found to occur for electron projectiles (6,7).

References

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