

Shape resonance spectrum of cytosine-guanine pairsM. T. do N. Varella*Instituto de Física, Universidade de São Paulo*

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Single and double strand breaks in DNA can be caused by low-energy electrons, the most abundant secondary products of the interaction of ionizing radiation to the biological matter. Attachment of these electrons to biomolecules lead to the formation of transient negative ions (TNIs) [1], often referred to as resonances, a process that may lead to significant vibrational excitation and dissociation. In the present study, we employ the parallel version [2] of the Schwinger Multichannel Method implemented with pseudopotentials [3] to obtain the shape resonance spectrum of cytosine-guanine (CG) pairs, with special attention to π^* transient anion states. Recent experimental studies pointed out a quasi-continuum vibrational excitation spectrum for electron collisions against formic acid dimers [4], suggesting that electron attachment into π^* valence orbitals could induce proton transfer in these dimers. In addition, our previous studies on the shape resonance spectra of the hydrogen-bonded complexes comprising formic acid and formamide units indicated interesting electron delocalization (localization) effects arising from the presence (absence) of inversion symmetry centers in the complexes [5]. In the present work, we extend the studies on hydrogen-bonded complexes to the CG pair, where localization of π^* anions would be expected, based on the previous results.

References

- [1]. B. Boudaïffa, P. Cloutier, D. Hunting, M. A. Huels, L. Sanche, *Science* 287, 1658 (2000).
- [2]. J. S. dos Santos, R. F. da Costa, M. T. do N. Varella, *J. Chem. Phys.* 136, 084307 (2012).
- [3]. M. H. F. Bettega, L. G. Ferreira, M. A. P. Lima, *Phys. Rev. A* 47, 1111 (1993).
- [4]. M. Allan, *Phys. Rev. Lett.* 98, 123201 (2007).
- [5]. T. C. Freitas, S. d'A. Sanchez, M. T. do N. Varella, M. H. F. Bettega, *Phys. Rev. A* 84, 062714 (2011).

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