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Research paper

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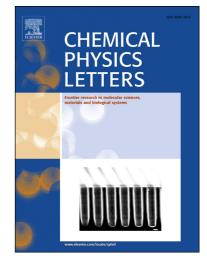
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Evolution of electron density towards the conical intersection of a nucleic acid purine

Luis Gutiérrez-Arzaluz, David Ramírez-Palma, Frida Buitrón-Cabrera, Tomás Rocha-Rinza, Fernando Cortés-Guzmán and Jorge Peón*

Institute of Chemistry, National Autonomous University of Mexico, Circuito Exterior, Ciudad Universitaria, Delegación Coyoacán C.P. 04510, Mexico

Abstract

We analyzed the evolution of the electron density across the S_0 and S_1 states potential energy curves of hypoxanthine (Hx) using the Quantum Theory of Atoms in Molecules (QTAIM). Examination of QTAIM energies and electronic populations indicates that charge transfer processes are important in the stabilization of the S_1 state towards the Conical Intersection (CI) which confers to Hx its photostability. Our results point that the rise of energy of the S_0 state approaching the CI is accompanied by a loss of aromaticity of hypoxanthine. Overall, the analyses presented herein give important insights on the photostability of nucleobases.

Keywords

DNA bases, excited states, TDDFT, Quantum Chemical Topology, electron density, conical intersections.

Introduction

Individual DNA bases have significant UV absorption cross sections of the order of 8 000 to $15\ 000\ M^{-1}\ cm^{-1}$. Despite this feature, these chromophores show an intrinsic photostability due to the presence of remarkable molecular mechanisms which efficiently eliminate the electronic energy associated with photon absorption.[1] Such mechanisms have been associated with natural selection processes at the molecular level which probably contributed to isolate highly photostable chromophores in the earliest stages of the evolution for organic compounds to make up the genetic material. [2–5]

The photostability of the four natural DNA bases and of several similar purines and pyrimidines is due to ultrafast photophysical processes in which one or a series of conical

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