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ORIGINAL ARTICLE

A systematic computational study of acridine derivatives through conceptual density functional theory

Prabhat Ranjan[1] · Brotati Chakraborty[2] · Tanmoy Chakraborty[3]

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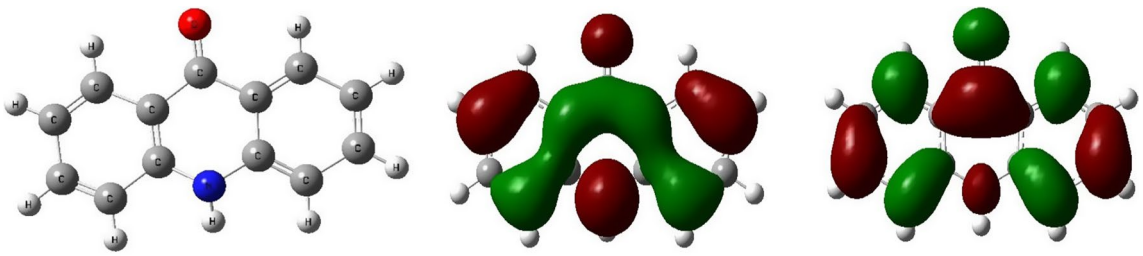
Abstract

A detailed computational analysis of acridine derivatives viz. acridone, 9-amino acridine hydrochloride hydrate, proflavin, acridine orange and acridine yellow is done in terms of conceptual density functional theory (CDFT). CDFT-based global descriptors—ionization potential, electron affinity, HOMO–LUMO gap, hardness, softness, electronegativity and electrophilicity index of acridine derivatives for ground state as well as excited state are estimated with the help of different hybrid functionals B3LYP/6-31G (d, p), B3LYP/6-311G (d, p), B3LYP/DGDZVP and B3LYP/LANL2DZ. Acridine derivatives show higher values of ionization potential and electron affinity in excited state as compared to ground state, indicating that these compounds are willing to accept electrons in excited state rather than donating electron. Acridone shows the maximum HOMO–LUMO energy gap in ground and excited state which implies that one-way electron transfer is most feasible with this compound. Our computed results emphasize the pronounced electron acceptor behaviour of the acridine derivatives in the excited state which has already been experimentally verified. It is observed that the trend in the computed values of the descriptors is not much improved on refinement of the basis set.

Graphical abstract



Keywords Density functional theory · Acridine derivatives · Electron affinity · Ionization potential · HOMO–LUMO gap

Introduction

Study of literature suggests that most of the research with acridine and its derivatives is focused on their interaction with deoxyribonucleic acid (DNA). Owing to its planar structure acridine is a typical DNA intercalator [1, 2]. The interaction of acridine derivatives with DNA is especially through electrostatic interaction and intercalation of the acridine moiety into DNA. This unique feature of acridine has been utilized to make use of acridine derivatives as DNA photo-footprinting agents [3], cytotoxic agent [4],

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