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ORIGINAL ARTICLE

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

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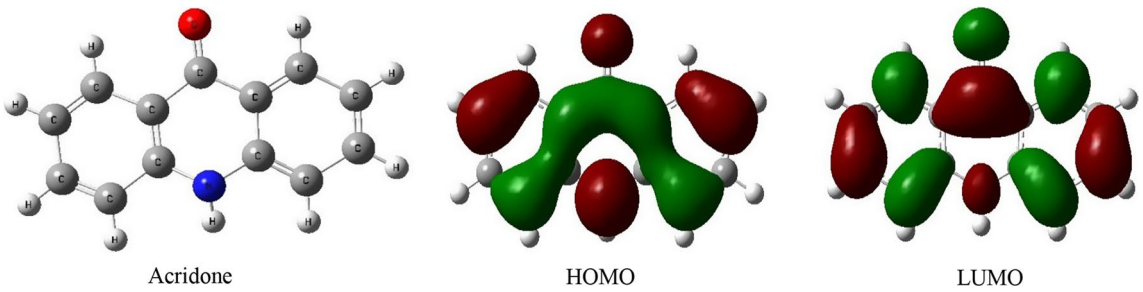
Abstract

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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telomere targeting agents [5–8] and also photocleaving agents [9, 10] of nucleic acids. Komiyama and co-workers prepared ribozyme mimics for "non-covalent" site-selective ribonucleic acid (RNA) scission by combining metal ions with DNA-acridine conjugates. When substrate RNA formed heteroduplexes with DNA-acridine conjugates, its phosphodiester linkage opposite the acridine was efficiently activated, and thus selectively hydrolysed by metal ions such as lanthanides (III), Zn (II) and Mn (II) [11–15]. Stein et al. showed that attachment of an acridine moiety to a catalytic tripeptide produced a RNase mimic [16]. There are very limited reports available in which interactions of acridine derivatives with proteins compared to that with DNA and RNA are discussed. The interaction of Proflavin (PF) with α-chymotrypsin and trypsin was extensively studied by a number of scientists [17–21]. Hanun and Bell observed that acridine orange (AO), acridine yellow (AY) and other related aminoacridines inhibited protein kinase C activity [22].

Some of the acridine derivatives like PF and AY are model photosensitizers in photodynamic therapy and have drawn the interest of researchers [23, 24]. Anti-cancer drug design considers DNA as one of its main targets. As acridine and its derivatives have the potential to bind to DNA via intercalation, so some of the acridine derivatives are considered to be prospective candidates in the treatment of cancer [25]. In fact, the prospect of acridine derivatives as chemotherapeutic agent and their antitumour as well as antiprotozoal activities have been explored by a number of workers [26, 27]. Although in cancer chemotherapy, the actual mechanism of drug action is complicated; however, exciting results were obtained during the study of mode of drug action with acridine derivatives. Identification and optimization of various acridine derivatives are required to increase the prospect of the members of the acridine family in the field of therapeutics and systematic computational studies may prove to be beneficial in such cases.

Although the application oriented study (i.e. the interactive study with DNA, RNA, proteins and other biological targets) of therapeutically important acridine derivatives is of immense significance, but the study of interaction of these members of acridine family with simple organic molecules also can be highly informative. In order to authenticate the participation of the acridine derivatives in fundamental processes like electron transfer (ET), proton transfer, hydrogen abstraction, etc., it is necessary to study the interaction of these compounds with simple organic moieties. For example, certain amines like *N,N′*-dimethylaniline (DMA), 4,4′-bis(dimethylamino)diphenylmethane (DMDPM), *N,N′*-diethylaniline (DEA), triethylamine (TEA), etc., classically serve as potent electron donors. Thus, to verify whether the acridine derivatives can act as electron acceptors in ET reactions, the interactions of the acridines with such organic amines may be investigated and later this information can possibly be utilized to explore similar roles of these acridines in their interactions with biologically relevant molecules. In other words, to study elementary processes like ET, proton transfer or hydrogen abstraction involving acridine derivatives and biologically relevant macromolecules, the study of interactions of these derivatives with simple organic molecules like aromatic and aliphatic amines is extremely essential.

The phenomenon of ET is ubiquitous in the field of chemistry and biology. If in an ET reaction either the acceptor or the donor moiety is in an excited state, then the process is called photoinduced electron transfer (PET) reaction. Radical or radical ions are produced in the due course of PET reactions, which may be affected by the existence of weak magnetic field (MF) of the order of 0.01–0.08 T. When such radicals/radical ions undergo diffusion in the medium and achieve an ideal separation where the exchange interaction becomes negligible, the internal MF produced by electron–nuclear hyperfine coupling can induce ample mixing of singlet (S) and triplet ($T_{\pm}$, T_0) spin states of the radical pair. Application of an external MF of the order of hyperfine interaction or higher can reduce such intersystem crossing by removing the degeneracy of the triplet states via Zeeman splitting leading to an increase in the population of the initial spin state of the radicals/radical ions [28, 29]. Laser flash photolysis (LFP) is one of the favourable techniques to directly probe non-fluorescent transients like radicals or radical ions by measurement of absorbance of such species.

A continuous attempt to spectroscopically probe the phenomenon of PET involving several acridine derivatives in chemically and biologically relevant systems, has been made since a decade [30–33]. ET involving various acridine derivatives like PF, AY, AO, 9-amionoacridine (9AA) and acridone (AD) have been studied in details using steady-state as well as time resolved fluorescence and LFP in conjunction with a weak MF. In the present communication, several physico-chemical properties of the acridine derivatives are computed and analysed invoking the exchange correlation B3LYP with different basis sets- 6-31G (d, p), 6-311G (d, p), DGDZVP and LANL2DZ within Density Functional Theory (DFT) framework. An effort has been made to correlate the theoretical findings with the experimental observations.

Methodology

DFT approach is considered to study the acridine derivatives. Conceptual Density Functional Theory (CDFT) is considered as one of the most popular computational techniques because it can easily describe and correlate experimental chemical properties in terms of CDFT-based descriptors. CDFT has marked its importance in the study of various

physico-chemical properties like electronic, optical, and magnetic properties, aromaticity, electronic stability and dynamics of chemical species [34–42]. In this report, acridine derivatives are investigated in terms of CDFT-based global descriptors. Geometry optimization and modelling are performed by using computational software Gaussian 16 within DFT framework [43]. Exchange correlation Becke-three parameter Lee-Yang-Parr (B3LYP) with different basis sets 6-31G (d, p), 6-311G (d, p), DGDZVP and LANL2DZ are chosen for geometry optimization. These basis sets and exchange correlational have been proven successful in computation of physico-chemical properties of acridine and its derivatives [44–50].

Ionization Potential (IP) and Electron Affinity (EA) of acridine derivatives are computed by using Koopman's theorem [34]:

$$\mathrm{IP} = -\varepsilon_{\mathrm{HOMO}} \tag{1}$$

$$\mathrm{EA} = -\varepsilon_{\mathrm{LUMO}} \tag{2}$$

The conceptual DFT-based descriptors-hardness (η), softness (S), electronegativity (χ) and electrophilicity index (ω) of acridine derivatives are computed as:

$$\chi = -\mu = \frac{\mathrm{IP} + \mathrm{EA}}{2} \tag{3}$$

where μ is the chemical potential of the system.

$$\eta = \frac{\mathrm{IP} - \mathrm{EA}}{2} \tag{4}$$

$$S = \frac{1}{2\eta} \tag{5}$$

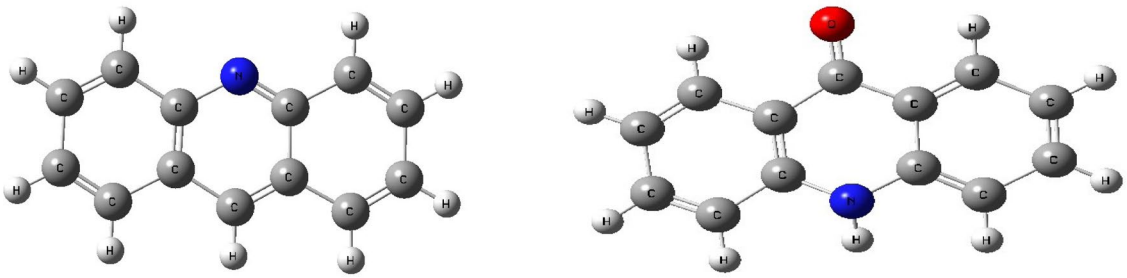
$$\omega = \frac{\mu^2}{2\eta} \tag{6}$$

Results and discussion

The structures of acridine derivatives are optimized within DFT framework and the optimized structures are presented in Fig. 1. Here all the structures of the acridine derivatives have real vibrational frequencies.

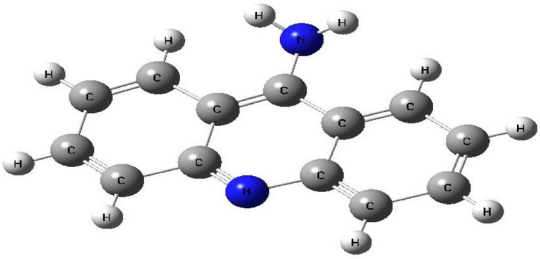
In an ET reaction, electron donor and electron acceptor are described with respect to the paired fragments. Electron donating behaviour is primarily determined based on IP of the molecule. In fact, a donor-acceptor complex consists of an electron donating molecule, characterized by its IP and an electron-accepting molecule, characterized by its EA. The IP as well as EA of acridine derivatives for ground state and excited state computed from different basis sets are presented in Tables 1 and 2, respectively. In the case of ground state, IP obtained from the basis set DGDZVP shows a higher value as compared to other basis sets except for AO. Similarly, except for PF and AO, EA calculated using DGDZVP has the highest value compared to other basis sets. Basis set 6-31G (d, p) shows the lowest IP and EA values for all the acridine derivatives, except AO. In the case of excited state, IP and EA obtained from basis set 6-311G (d, p) is the maximum in comparison with other basis set data except for AD and 9AA. It is observed from Tables 1 and 2 that IP and EA in excited state is much higher in comparison with that in the ground state for the acridine derivatives, which means that in excited state they are reluctant to donate electron, rather they are willing to accept electron. It is to be noted that increase in the value of EA on going from ground to excited state is most prominent for AD and 9AA implying that they can act as very good electron acceptor in the excited state. The fact that AD can act as an electron acceptor has already been verified experimentally while studying the interaction of AD with various classical electron donors like DMA, DEA, TEA, etc. [51], and also with tryptophan residues embedded in the biological nanocavities of HSA [52] and BSA [53]. Moreover, it is also verified that 9AA can act as a potent electron acceptor while studying ET reactions involving 9AA and DMA as well as TEA [54]. The EA values of 9AA and AY are significantly low in the ground state as evident from Table 1. This points to the fact that 9AA can act as an electron donor to an acceptor in the excited state. The electron donating capacity of 9AA has been explored while studying its interaction with methylviologen [55]. It is observed that IP and EA values of acridine and AD do not change significantly on varying the basis sets and the trend in the values of these two parameters for the acridine derivatives discussed in this article is also not appreciably changed on changing the basis set.

Highest Occupied Molecular Orbital (HOMO)—Lowest Unoccupied Molecular Orbital (LUMO) gap of acridine derivatives for ground state and excited state are presented in Figs. 2 and 3, respectively. AD and PF show maximum and minimum HOMO–LUMO gap, respectively, in the case of ground state as depicted in Fig. 2. Higher HOMO–LUMO gap implies a greater stability due to the maximum hardness principle [56, 57]. It may be noted that HOMO–LUMO gap for AD is the highest among all the listed molecules both in ground and excited state implying that one-way electron transfer is most feasible with this molecule. Thus, AD in excited state is a better electron acceptor in comparison with the other acridine derivatives discussed in the present study. This may somewhat be attributed to the carbonyl group present in the molecule which makes it a strong electron acceptor similar to other such molecules bearing same functional group like menadione, anthraquinone, etc. [58,

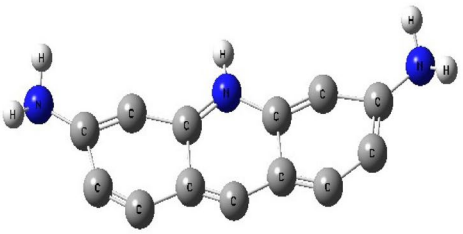


(a) Acridine

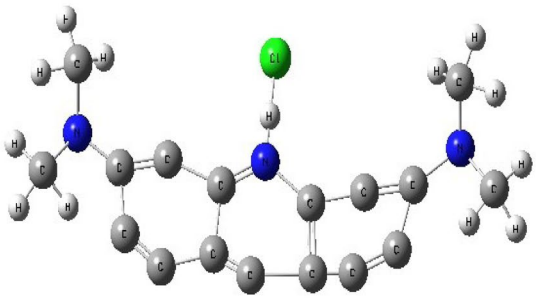
(b) Acridone



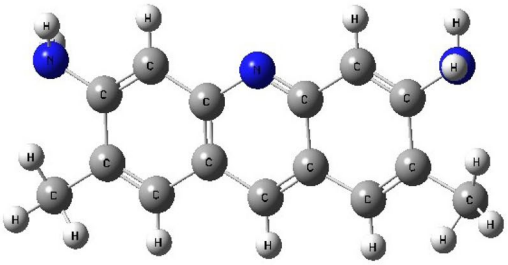
(c) 9-amino acridine hydrochloride hydrate



(d) Proflavin



(e) Acridine Orange



(f) AcridineYellow

Fig. 1 Optimized structure of acridine derivatives

Table 1 Ionization potential and electron affinity of acridine derivatives for ground state

Species	6-31G (d, p)		6-311G (d, p)		DGDZVP		LANL2DZ	
	IP	EA	IP	EA	IP	EA	IP	EA
Acridine	5.717	2.015	5.963	2.260	5.971	2.324	5.891	2.254
Acridone	5.684	1.614	5.921	1.875	5.935	1.923	5.881	1.895
9-Amino acridine hydrochloride hydrate	5.098	1.583	5.344	1.838	5.522	2.047	5.310	1.861
Proflavin	5.286	3.895	5.607	4.164	5.831	4.315	5.698	4.383
Acridine orange	5.362	3.665	5.618	4.152	5.124	1.712	2.976	0.099
Acridine yellow	4.693	1.223	4.930	1.461	5.213	1.695	4.872	1.442

Table 2 Ionization potential and electron affinity of acridine derivatives for excited state

Species	6-31G (d, p)		6-311G (d, p)		DGDZVP		LANL2DZ	
	IP	EA	IP	EA	IP	EA	IP	EA
Acridine	10.462	6.953	10.641	7.139	10.623	7.136	10.578	7.123
Acridone	10.621	6.105	10.802	6.298	10.745	6.271	10.752	6.300
9-Amino acridine hydrochloride hydrate	9.809	6.322	9.995	6.514	8.092	5.471	9.951	6.524
Proflavin	9.789	7.010	9.986	7.237	8.082	6.062	10.101	7.063
Acridine orange	8.765	5.719	8.847	5.897	7.161	5.481	4.870	1.443
Acridine yellow	6.384	3.512	6.604	4.168	6.663	3.823	6.566	3.701

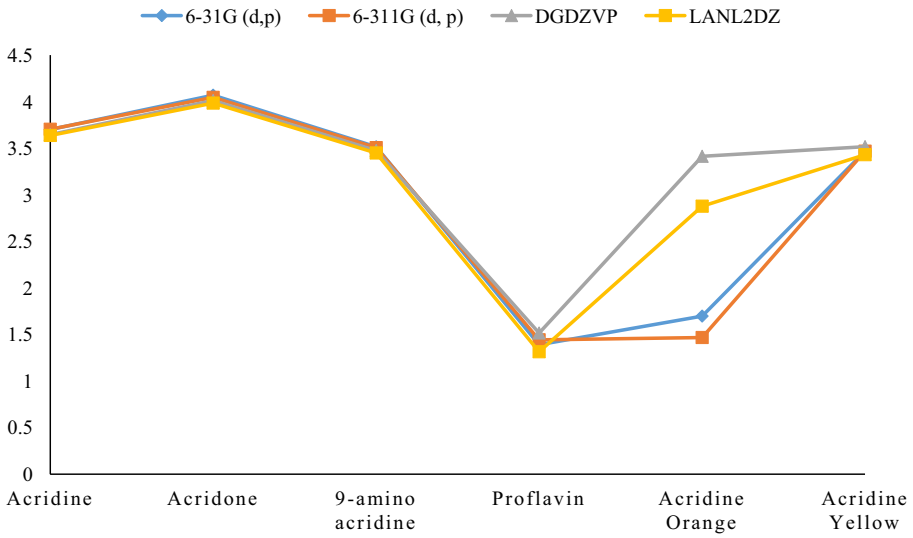


Fig. 2 HOMO–LUMO gap (in eV) for ground state

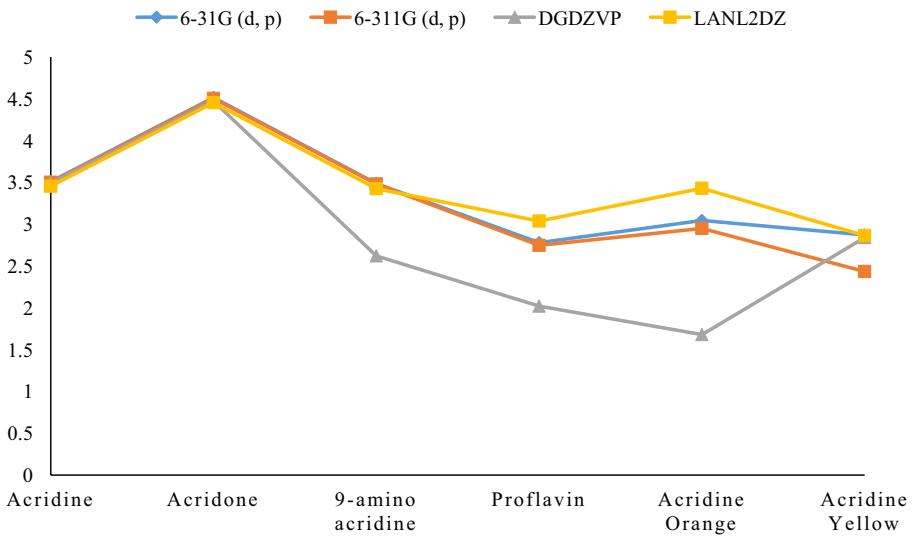


Fig. 3 HOMO–LUMO gap (in eV) for excited state

59]. It is observed that in the ground state for acridine, basis set 6-311G (d, p) provides the maximum HOMO–LUMO gap, for AD and 9AA the maximum gap is witnessed by the basis set 6-31G (d, p) and for PF, AO and AY maximum HOMO–LUMO is seen in the case of basis set DGDZVP. On the contrary, in the excited state, basis set 6-31G (d, p) provides the maximum HOMO–LUMO gap for species acridine, AD, 9AA and AY whereas basis set LANL2DZ

offers the maximum HOMO–LUMO gap for PF and AO. HOMO–LUMO gap for acridine and AD is independent of the basis set used in the ground as well as excited state as depicted in Figs 2 and 3. Frontier orbitals-HOMO and LUMO of acridine derivatives for ground state obtained from basis sets—DGDZVP and LANL2DZ are shown in Figs. 4 and 5, respectively.

Molecular hardness and softness of these molecules for ground state as well as excited state are computed and presented in Tables 3 and 4, respectively. Molecular hardness and softness are related to the kinetic stability of chemical species. It is reported that chemical species with high value of HOMO–LUMO gap shows high value of molecular hardness and least softness value [60–62]. The data reveals that

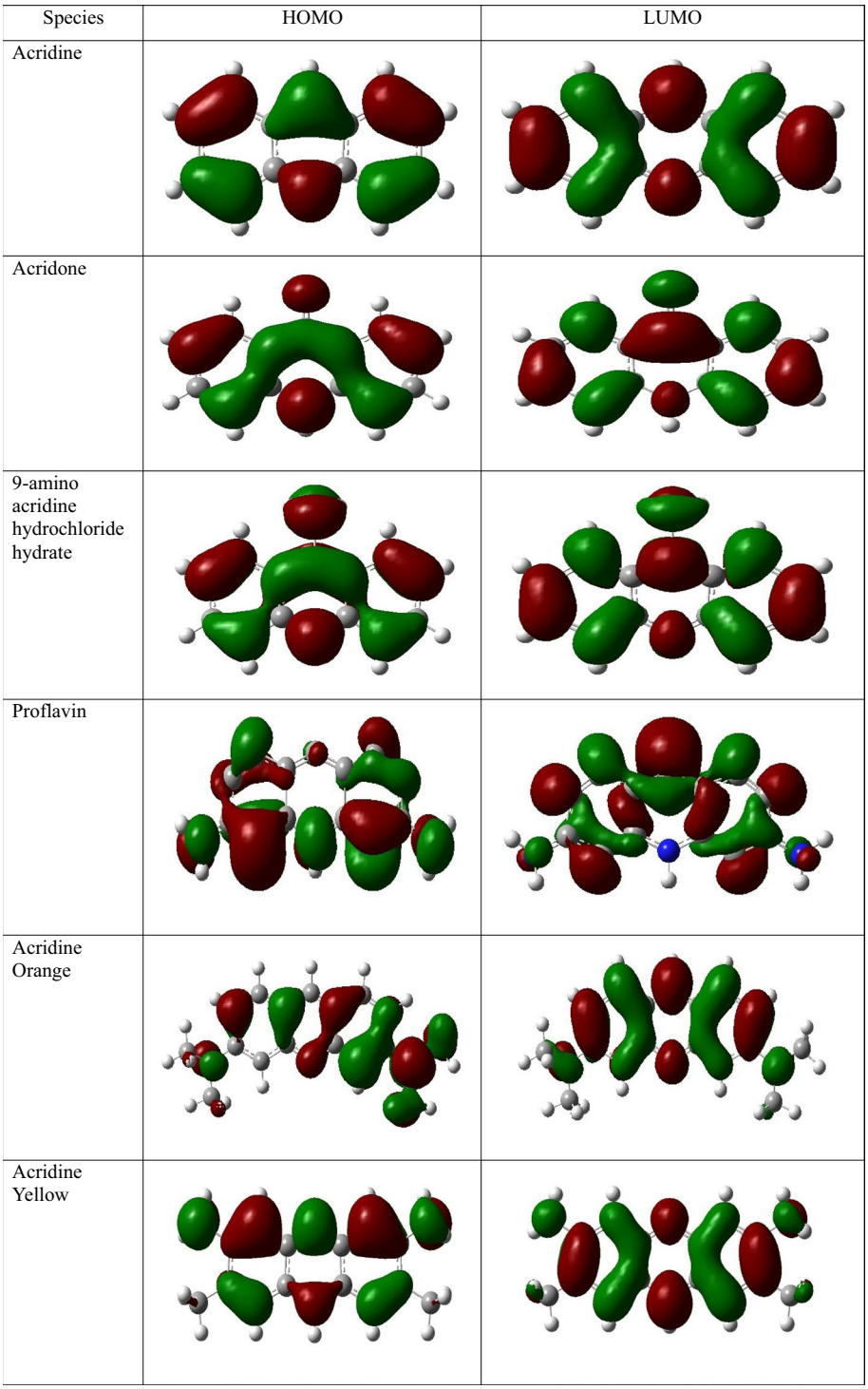


Fig. 4 HOMO and LUMO of acridine derivatives for ground state using basis set DGDZVP

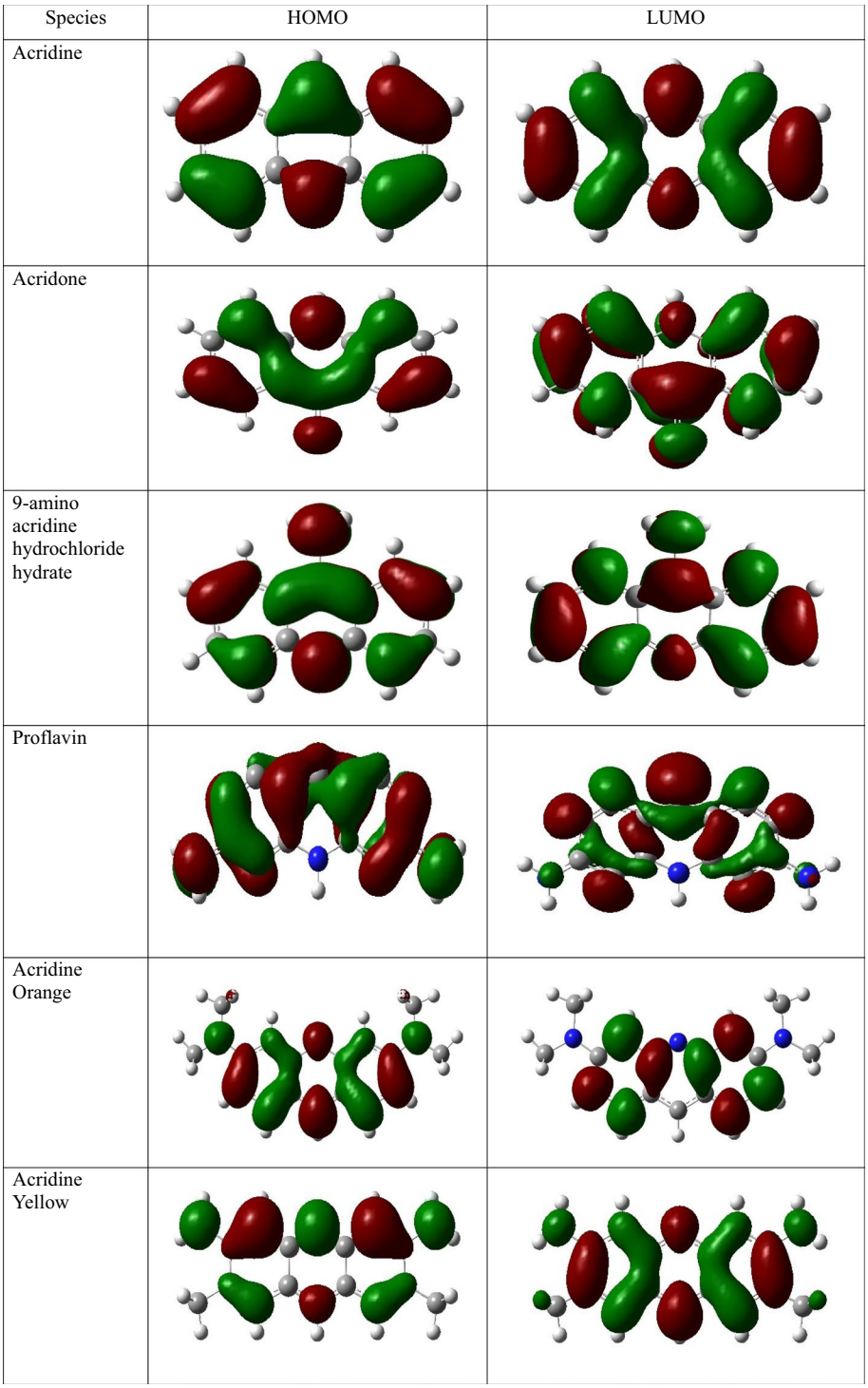


Fig. 5 HOMO and LUMO of acridine derivatives for ground state using basis set LANL2DZ

among all these acridine derivatives AD and PF are having maximum and minimum stability, respectively. In ground state, basis set 6-311G (d, p) provides the maximum hardness for species acridine. For AD and 9AA, the maximum hardness is produced by basis set 631G (d, p) whereas basis set DGDZVP provides the maximum hardness for PF, AO and AY. On the contrary, basis set LANL2DZ provides the maximum softness value for compounds acridine, AD, 9AA, PF and AY whereas 6-311G (d, p) offers the maximum softness value for AO in the case of ground state. Hardness and softness values in the ground state show no discrepancy on the choice of basis set for acrdine, AD and 9AA while for excited state no discrepancy is found on change of basis set for acridine and AD.

Electronegativity and electrophilicity index of acridine derivatives for ground as well as excited state are listed in Tables 5 and 6, respectively. During the interaction of two chemical species electrons begin to move towards species having higher electronegativity from that having lower electronegativity. This trend will remain until the electronegativity of donor, acceptor and adduct reaches a threshold [60, 63]. PF shows the highest electronegativity value in the ground state whereas in excited state acridine displays the maximum value. It is evident from Tables 5 and 6 that electronegativity value in the excited state is much greater in comparison with the ground state for all the acridine derivatives discussed in this article. In the ground state, basis set DGDZVP provides the maximum value of electronegativity for acridine, AD, 9AA, PF and AY whereas 6-311G (d, p) offers the maximum electronegativity for AO.

The first theoretical definition of electrophilicity index as was proposed by Parr et al. [36]. They described it as a system's ability to "soak up" electrons. It is observed that HOMO–LUMO gap is lower in case of PF, AO and AY in comparison with other molecules listed in the figures, implying they can easily donate or accept electron with respect to counter molecule. However, compared to ground state PF and AY have greater electrophilicity in the excited state, which means they are more eager to accept electron in excited state compared to their ground states; whereas in case of AO we do not find remarkable change in electrophilicity, which means in excited state AO does not favour

Table 3 Hardness (η) and softness (S) for ground state

Species	6-31G (d, p)		6-311G (d, p)		DGDZVP		LANL2DZ	
	η	S	η	S	η	S	η	S
Acridine	1.851	0.270	1.852	0.270	1.823	0.274	1.818	0.275
Acridone	2.035	0.246	2.023	0.247	2.006	0.249	1.992	0.251
9-Amino acridine hydrochloride hydrate	1.758	0.284	1.753	0.285	1.738	0.288	1.724	0.290
Proflavin	0.695	0.719	0.722	0.693	0.758	0.660	0.658	0.760
Acridine orange	0.848	0.589	0.733	0.682	1.707	0.293	1.438	0.348
Acridine yellow	1.735	0.288	1.734	0.288	1.757	0.284	1.715	0.292

Table 4 Hardness (η) and softness (S) for excited state

Species	6-31G (d, p)		6-311G (d, p)		DGDZVP		LANL2DZ	
	η	S	η	S	η	S	η	S
Acridine	1.755	0.285	1.751	0.286	1.744	0.287	1.728	0.289
Acridone	2.258	0.221	2.252	0.222	2.237	0.224	2.226	0.225
9-Amino acridine hydrochloride hydrate	1.743	0.287	1.741	0.287	1.311	0.382	1.713	0.292
Proflavin	1.390	0.360	1.374	0.364	1.010	0.495	1.519	0.329
Acridine Orange	1.523	0.328	1.475	0.339	0.840	0.595	1.715	0.291
Acridine Yellow	1.436	0.348	1.218	0.411	1.420	0.352	1.432	0.348

Table 5 Electronegativity (χ) and electrophilicity index (ω) for ground state

Species	6-31G (d, p)		6-311G (d, p)		DGDZVP		LANL2DZ	
	χ	ω	χ	ω	χ	ω	χ	Ω
Acridine	3.867	4.039	4.112	4.566	4.148	4.718	4.073	4.562
Acridone	3.650	3.273	3.899	3.757	3.930	3.849	3.888	3.794
9-Amino acridine hydrochloride hydrate	3.341	3.175	3.592	3.679	3.785	4.122	3.586	3.728
Proflavin	4.591	15.160	4.886	16.536	5.073	16.976	5.041	19.324
Acridine orange	4.514	12.009	4.825	16.275	3.418	3.423	1.538	0.822
Acridine yellow	2.958	2.523	3.196	2.945	3.453	3.393	3.157	2.907

Table 6 Electronegativity (χ) and electrophilicity index (ω) for excited state

Species	6-31G (d, p)		6-311G (d, p)		DGDZVP		LANL2DZ	
	χ	ω	χ	ω	χ	ω	χ	Ω
Acridine	8.708	21.610	8.891	22.571	8.880	22.612	8.851	22.673
Acridone	8.364	16.233	8.550	16.233	8.508	16.183	8.527	16.328
9-Amino acridine hydrochloride hydrate	8.066	18.657	8.255	19.573	6.782	17.546	8.237	19.809
Proflavin	8.400	25.387	8.612	26.987	7.072	24.755	8.582	24.241
Acridine orange	7.242	17.218	7.373	18.425	6.321	23.777	3.156	2.908
Acridine yellow	4.949	8.526	5.386	11.913	5.244	9.681	5.134	9.200

acceptance of electron as much as PF or AY. Electrophilicity of all the compounds except AO increases notably in the excited state indicating that the acridine derivatives behaves as a better electron acceptor in the excited state. Electrophilicity index is higher in the excited state, as expected from the minimum electrophilicity principle [64–66]. The role of PF as an electron acceptor in ET reactions has already been studied while exploring its interaction with TEA [30, 67], DMA and DMDPM [31, 67] and also tryptophan residue confined in a reverse micelle [68] as well as that housed in HSA [32]. In fact, PF is also found to behave as an electron acceptor while interacting with DNA [69]. Similarly, AY also behaves as an electron acceptor while interacting with classical electron donors like DMA, DMDPM and TEA [33] as well as DNA [69], which has been experimentally verified using spectroscopic techniques. Although no reports till date suggests that PF and AY can act as electron donors in ET reactions, however, their corresponding radical anion have been found to serve as potential electron donor which can transfer electron to classical electron acceptors like methyl viologen and others [70]. The theoretical finding that AO is reluctant to accept electron in the excited state unlike PF and AY has been experimentally noticed while investigating the interaction of a AY, PF and AO with DNA [69]. In fact, AO shows a distinctly different observation in the fluorescence lifetime study in comparison with PF and AY on addition of DNA, indicating its unwillingness to accept electron in the excited state. For ground state, basis set DGDZVP offers the maximum electrophilicity index for acridine, AD, 9AA and AY whereas for species PF and AO the highest electrophilicity indices are produced by LANL2DZ and 6-311G (d, p), respectively. It may be noted from Tables 5 and 6 that for compounds like AD, the values of electronegativity in both ground and excited states are not much changed on varying the basis set. Further, the trend of electronegativity and electrophilicity indices for all the compounds are also not appreciably altered on changing the basis set.

Dipole moment (in Debye) of these acridine derivatives for ground state as well as excited state are shown in Figs. 6 and 7, respectively. The result shows that AD has the maximum whereas AY has the least value of dipole moment among all these derivatives in ground state. However, in the excited state AY displays the maximum dipole moment. In fact, while studying the interaction of AY

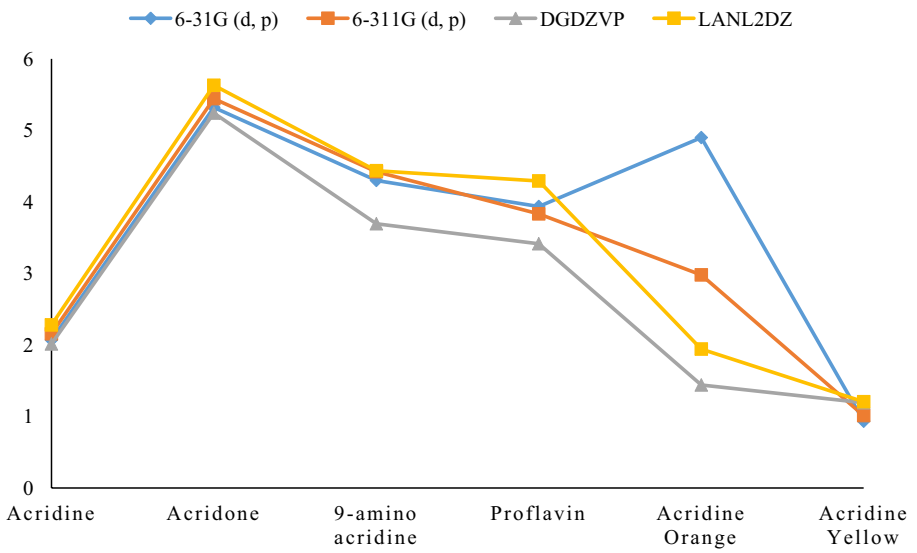


Fig. 6 Dipole moment (in Debye) for ground state

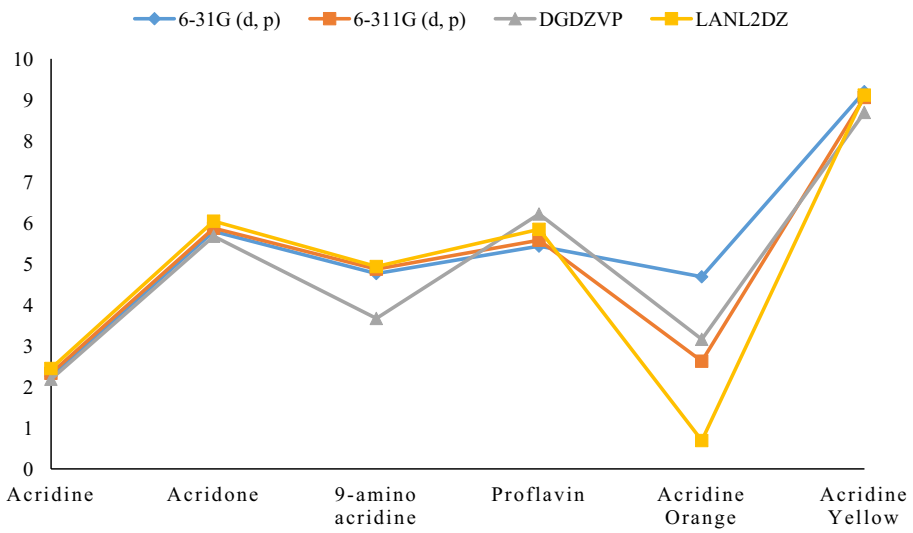


Fig. 7 Dipole moment (in Debye) for excited state

with Cucurbit[7]uril, we have rationalized the discrepancies in the results obtained from calorimetric and spectroscopic techniques in the light of remarkable increase in dipole moment of AY on excitation [71]. In Table 7, dipole moments for some of the acridine derivatives are compared with available experimental and theoretical data [72]. In general, computed data is in agreement with the reported values. It is reported that in the excited state the value of dipole moment is high in comparison with ground state [72] and similar pattern is visible from our calculated data. Aaron et al. [72] reported the values of dipole moment of some acridine derivatives and found that difference in the values of dipole moment for excited state and ground state is large, especially in the case of PF due to intense solute-solvent relations. The data reveal that in ground state, the basis set LANL2DZ provides the maximum dipole moment for species acridine, AD, 9AA, PF and AY whereas 6-31G (d, p) offers the maximum dipole moment for AO.

Conclusion

Theoretical analyses of acridine and its derivatives like PF, AY, AO, 9AA and AD are done by using DFT methodology. CDFT-based descriptors viz. ionization potential, electron affinity, HOMO–LUMO gap, molecular hardness, softness, electronegativity and electrophilicity index are estimated for ground as well as excited states of these compounds by using exchange correlation B3LYP with different basis sets: 6-31G (d, p), 6-311G (d, p), DGDZVP and LANL2DZ. IP and EA of acridine derivatives show higher values in excited state as compared to the ground state. It indicates that in excited state these compounds are reluctant to donate electron and willing to accept electron. The values of EA for AD and 9AA have increasing trend while moving from ground to excited state which is in line with the experimental results. It implies that compounds AD and 9AA can act as very good electron acceptor in the excited state. The HOMO–LUMO energy gap for AD is the maximum in ground as well as excited states showing that one-way electron transfer is most feasible with this compound. For all the acridine derivatives

Table 7 Comparison between computed and experimental dipole moments of some acridine derivatives in Debye

Species	Ground state		Excited state	
	Computed data, 6-311G (d, p)	Experimental and theoretical data [72]	Computed data, 6-311G (d, p)	Experimental and theoretical data [72]
Acridine	2.156	2.99[a], 2.33[b]	2.331	6.6[a], 1.56[b]
9-Amino acridine hydrochloride hydrate	4.421	5.23[a], 5.19[b]	4.872	7.1[a], 4.59[b]
Proflavin	3.833	3.96[a], 2.90[b]	5.577	8.7[a], 1.46[b]
Acridine yellow	1.012	6.33[a], 5.19[b]	9.058	9.8[a], 2.95[b]

[a]Experimental data, [b]Theoretical data

discussed in this article, electronegativity value is larger in the excited state than in the ground state. Electrophilicity index of all the compounds except AO increases notably in the excited state indicating that the acridine derivatives behave as a better electron acceptor in the excited state. The computed findings correspond the experimental data closely. It is pertinent to mention here that although the CDFT-based descriptors of acrdine and its derivatives are computed using a number of basis sets, in most of the cases it is observed that the trend in the values of the computed parameters are similar on varying the basis set. There is a good agreement in the trend of CDFT-based parameters of the listed compounds by changing the basis set. This implies that trend in the computed values of the descriptors is not much improved on refinement of the basis set. Further, for some molecules like AD, the values of the CDFT-based descriptors are almost independent of the basis set used.

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Declarations

Conflict of interest The authors declare no conflict of interest.

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