

Fluorescence and solvatochromic studies of biologically important Schiff base derivatives

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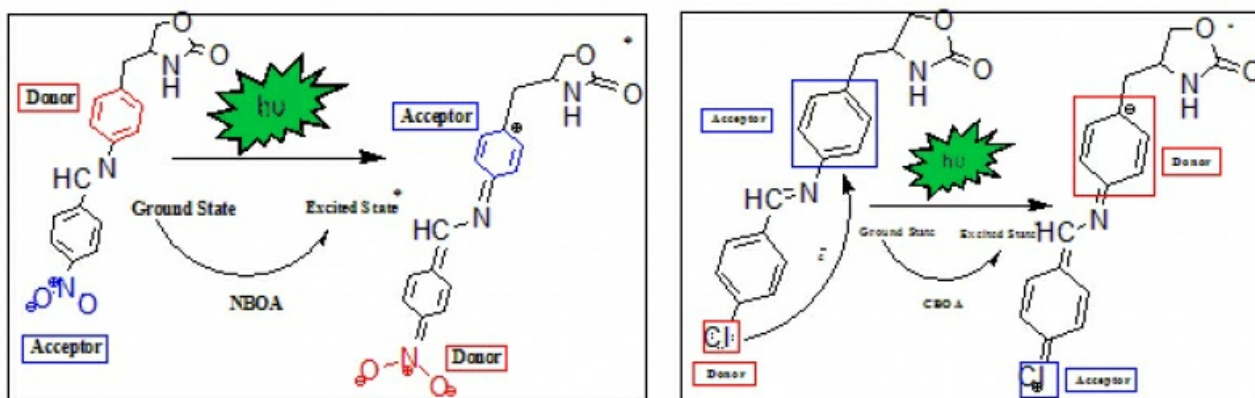
Schiff bases have extensive applications in therapeutic and optoelectronic fields. Schiff bases have shown significant optical properties and used as photochromic compound, light emitting diode, nonlinear optical materials, optical and electrochemical sensors.

In the present investigation, we report detail study on photophysical properties of two Schiff base derivatives. Absorption and fluorescence studies on novel Schiff bases (E)-4-(4-(4-nitrobenzylideneamino)benzyl)oxazolidin-2-one (NBOA) and (E)-4-(4-(4-chlorobenzylideneamino)benzyl)oxazolidin-2-one (CBOA) have been performed in a series of solvents of increasing polarity at room temperature. Large Stokes shift shows bathochromic red-shift for fluorescence band in both the ligands. The substituents in Schiff base help to understand the intramolecular charge transfer processes. Electron donating substituent contributes large extent of ICT and positive solvatochromism compared to electron withdrawing one. Ground-state and singlet excited-state dipole moments of NBOA and CBOA have been calculated experimentally using Lippert-Mataga, Bakhshiev, Kawskii-Chamma-Viallet, and Reichardt methods. The singlet excited-state dipole moment was found to be greater than that of the ground-state. Kamlet-Abboud-Taft and Catalan multiple linear regression approaches were used to get detailed information of both non-specific solute-solvent interaction and hydrogen bonding interactions. Optimized geometry and HOMO-LUMO energies of NBOA and CBOA have been determined by TD-DFT (B3LYP/6-311G (d, p)). Mulliken charges and molecular electrostatic potential have also been evaluated from DFT calculations.

[1] Acemioglu B. et al. (2001) J. Mol. Struct. (Theochem) 548, 165-171.

[2] Siddlingeshwar B. et al. (2009) Spectrochim. Acta A. 72, 490-495.

[3] Melavanki R. M. et al. (2012) J. Fluoresc. 22, 137-144.



Intramolecular charge transfer of NBOA and CBOA

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