# A Comprehensive Spectroscopic and Computational Investigation of Intramolecular Proton Transfer in the Excited States of 2-(2'-Hydroxyphenyl) Benzoxazole and its Derivatives

V. Padalkar[1], P. Ramasami[2]* and N. Sekar[1]*

[1]*Tinctorial Chemistry Group, Department of Dyestuff Technology, Institute of Chemical Technology, Matunga, Mumbai-400019, India*
[2]*Computational Chemistry Group, Department of Chemistry, Faculty of Science, University of Mauritius, Réduit, Mauritius*

*Authors for correspondence e-mails: n.sekar@ictmumbai.edu.in, ramchemi@intnet.mu

The excited-state intramolecular proton transfer (ESIPT) fluorescence of the 2-(2' hydroxyphenyl) benzoxazole (HBO) and its derivatives was studied by spectroscopic and computational methods. The changes in the electronic transition, energy levels, and orbital diagrams of the HBO derivatives were investigated using the DFT computations and they were correlated with the experimental spectral emission. The benzoxazole derivatives are fluorescent under UV-light in solution. Photophysical properties of the compounds were also studied in solvents of different polarities. Experimental absorption and emission wavelengths are in agreement with the computed one with a deviation ranging between 0 and 50%. The computational methods have been useful for molecular understanding of the transitions responsible for the fluorescent spectra. ESIPT process of studied compounds is shown in following figure.