Red Emitting Coumarins: Insights of Photophysical Properties with DFT Calculations

A. B. Tathe and N. Sekar*

Tinctorial Chemistry Group, Department of Dyestuff Technology, Institute of Chemical Technology, N. P. Marg, Matunga, Mumbai, India

*Author for correspondence e-mails: nethi.sekar@gmail.com, n.sekar@ictmumbai.edu.in

Red emitting dyes are of great interest in various technological applications. Coumarins, though being an important class of fluorescent molecules have been rarely studied for the red emission. The structural and electronic aspects of three red emitting coumarins have been studied using DFT and TDDFT methods. The functionals employed are the hybrid functionals B3LYP, CAM-B3LYP, PBE0 and highly parameterized empirical functional M06. Pople's basis sets with added polarization and diffusion functions were benchmarked for their performance with these molecules. The vertical excitations obtained theoretically with PCM solvation model were compared with those observed in various solvents. The rationale of the red shifted absorption is established. The B3LYP functional was proved to be the best one to estimate vertical excitation and predicts with ~10% deviation. The basis set effect on the accuracy of the results is almost nil and majorly depends on the functional selected.

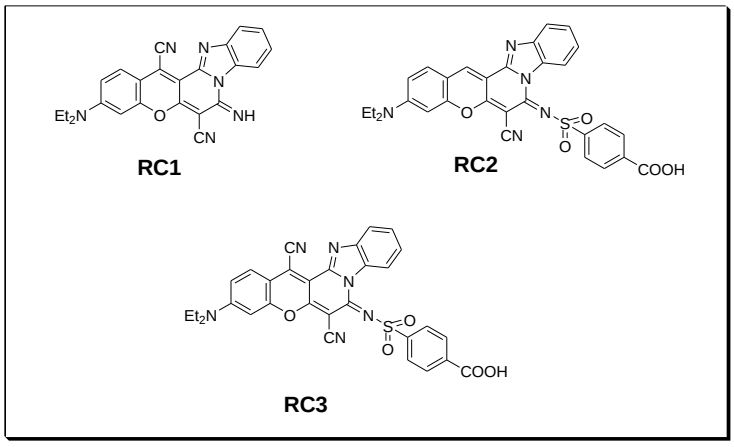

Figure 1: Red emitting coumarins.