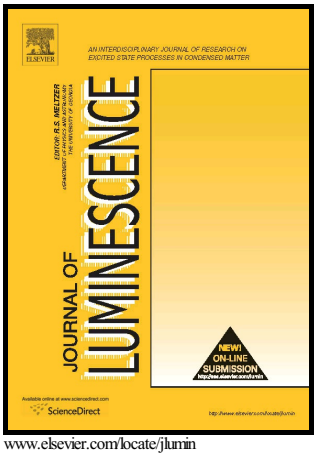

www.elsevier.com/locate/jlumin

Deciphering the Perturbation Effect of Urea on the Supramolecular Host-Guest Interaction of Biologically Active Hydrophobic Molecule inside the Nanocavity of Cyclodextrins

Banibrata Maity, Aninda Chatterjee, Sayeed Ashique Ahmed, Debabrata Seth

PII: S0022-2313(16)30691-3
DOI: http://dx.doi.org/10.1016/j.jlumin.2016.11.037
Reference: LUMIN14375

To appear in: *Journal of Luminescence*

Received date: 28 May 2016
Revised date: 15 September 2016
Accepted date: 15 November 2016

Cite this article as: Banibrata Maity, Aninda Chatterjee, Sayeed Ashique Ahmed and Debabrata Seth, Deciphering the Perturbation Effect of Urea on the Supramolecular Host-Guest Interaction of Biologically Active Hydrophobic Molecule inside the Nanocavity of Cyclodextrins, *Journal of Luminescence* http://dx.doi.org/10.1016/j.jlumin.2016.11.037

Deciphering the Perturbation Effect of Urea on the Supramolecular Host-Guest Interaction of Biologically Active Hydrophobic Molecule inside the Nanocavity of Cyclodextrins

Banibrata Maity, Aninda Chatterjee, Sayeed Ashique Ahmed, Debabrata Seth*

Department of Chemistry, Indian Institute of Technology Patna, Patna 801103, Bihar, India

debabrata@iitp.ac.in; Phone: 91-612-3028028

ABSTRACT

The present work articulates the supramolecular interaction and the formation of host-guest complex between the biologically active hydrophobic coumarin derivative and cyclodextrins by using several spectroscopic, calorimetric and microscopic techniques. All the studies clearly revealed that in presence of cyclodextrins (CDs), coumarin forms 1:1 stoichiometric complex. From all the study, we have found that with gradual increasing the cavity diameter of the hosts, the binding efficiency of the complexes gradually increases. The small population of the non emissive twisted intramolecular charge transfer (TICT) state of coumarin molecule turns into highly emissive in presence of γ-CD owing to its greater cavity diameter. The emissive TICT band is not found in β-CD complex due to its comparative small hydrophilic exterior and less polar environment. The present finding also interpret the perturbation effect of urea on host-guest complexes. In the presence of urea, the TICT emissive band of γ-CD is completely diminished. From, ^{1}H-NMR study it was observed that $-NEt_2$ moiety of 7-DCCAE molecule is deeply buried inside the hydrophobic cavity of the CDs and forms host-guest complexes. Isothermal titration calorimetry measurement also indicates the formation of 1:1 host-guest complexes.

Keywords: Host-guest complex, isothermal titration calorimetry, fluorescence spectroscopy, twisted intramolecular charge transfer.