Electronic Supplementary Material (ESI) for Photochemical & Photobiological Sciences

Encapsulation of 2-(4'-*N*,*N*-dimethylamino)phenylimidazo[4,5-*b*]pyridine in β-cyclodextrin: Effect on H-bond induced intramolecular charge transfer emission

Nihar Dash, Francis A. S. Chipem and G. Krishnamoorthy*
Department of Chemistry
Indian Institute of Technology Guwahati
Guwahati 781039
India

^{1}H NMR in $CDCl_3$ and assignment of protons

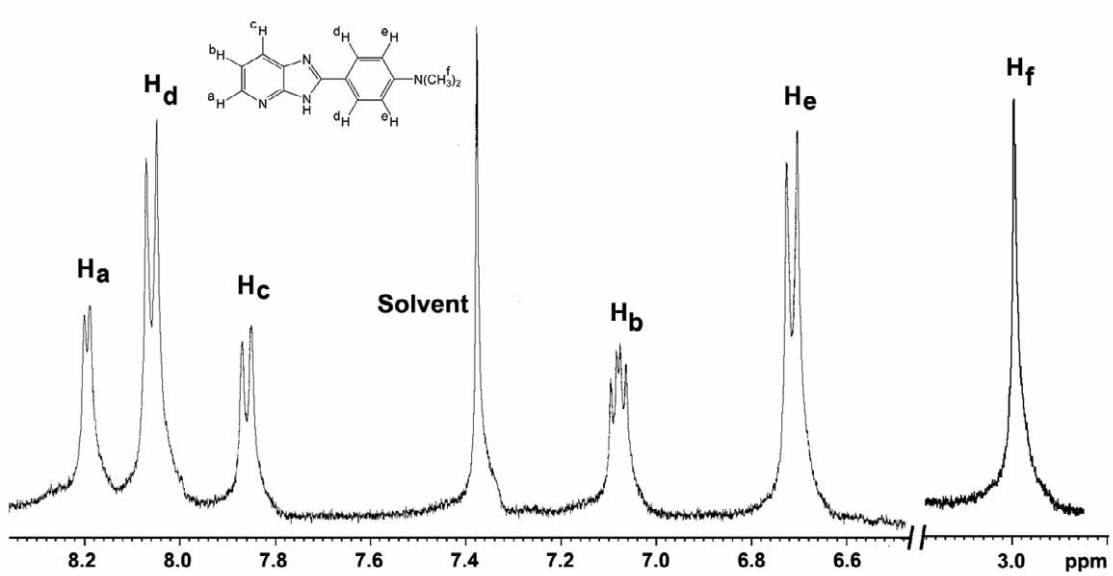

Figure: ^{1}H NMR spectrum of DMAPIP-b in $CDCl_3$ (intensity of aromatic region is expanded approximately by a factor of six).

Assignment of protons in the aromatic region

$\mathbf{H_a}$, $\mathbf{H_c}$ type protons expected to be a doublet due to splitting of neighboring $\mathbf{H_b}$ proton, and $\mathbf{H_a}$ is expected in down field due to the presence of neighboring hereto atom. Accordingly δ 8.24 (d, J = 5 Hz , 1H) and 7.96 (dd, J = 8, 5 Hz, 1H) can be assigned to $\mathbf{H_a}$ and $\mathbf{H_c}$ respectively.

$\mathbf{H_b}$ is expected to be doublet of doublet, only doublet of doublet at δ 7.14 (dd, J = 8, 5 Hz, 1H) thus corresponds to $\mathbf{H_b}$.

H_d, **H_e** type protons expected to be a doublet due to splitting of neighboring proton of other type i.e. **H_d** by **H_e** and **H_d** by **H_e**. **H_d** is expected in downfield (compare to **H_e**) due to the presence of neighboring heterocylic ring. Thus δ 8.12 (d, J = 9 Hz, 2H) and 6.74 (d, J = 9 Hz, 2H) can be assigned to **H_d** and **H_e** types of protons respectively.

The assignments were further substantiated by the decoupled spectra shown below.

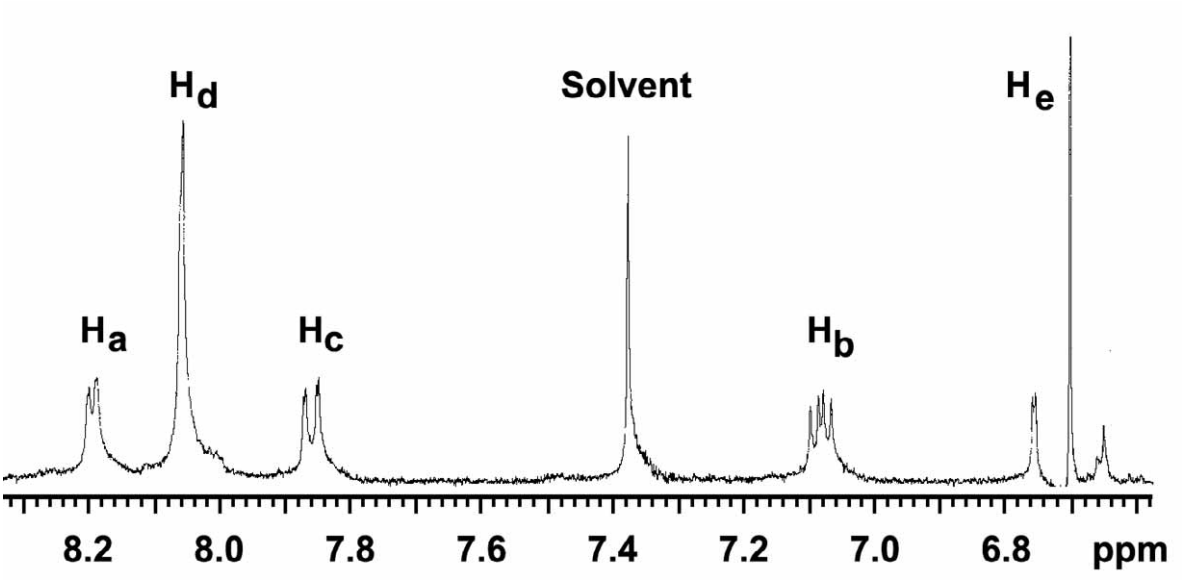

Figure: H_f protons decoupled aromatic region of ^{1}H NMR spectrum of DMAPIP-b in $CDCl_3$.

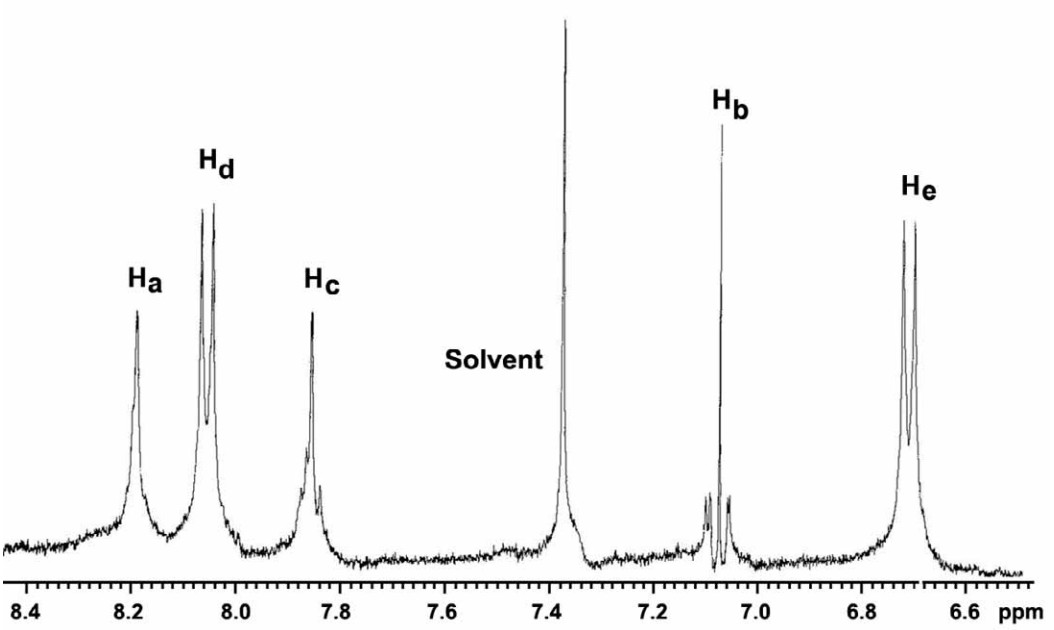

Figure: H_b proton decoupled aromatic region of ^1H NMR spectrum of DMAPIP-b in $CDCl_3$.