Ain Shams University
Faculty of Science
Chemistry Department

Effect of inclusion in cyclodextrin nanocavities on the excited state proton transfer of photoacids.

A Thesis
Submitted for the Degree of Master of Science
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"Chemistry Department"
By

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2013

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Approval Sheet

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Aya Said Amer

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List of symbols

Symbol	Scientific meaning
A	Absorbance
$h\nu$	Energy
AH	BrØnsted acid
B	BrØnsted base
BH^+	Conjugate acid
A^-	Conjugate base
k_{IC}	Internal conversion rate constant
k_{ISC}	Inter system crossing rate constant
k_F	Fluorescence rate constant
k_P	Phosphorescence rate constant
k_{ext}	Excitation rate constant
ν_a	Absorption energy
ν_F	Fluorescence energy
$\Delta\nu$	Stokes shift
I_o	Intensity of fluorescence decay at zero time
I(t)	Intensity of fluorescence decay at any time
ε	Dielectric constant

a, b, p, s, d, di and e	Susceptibility constants
D	Guest molecule
I_f ,I_f^o	Fluorescence intensity in the presence and absence of cyclodextrin
I_C	Fluorescence intensity of the guest-CD complex
μ_g / μ_e	Ground state and excited state dipole moment
k_r	Radiative rate constant
k_{nr}	Non-radiative rate constant
k_q	Quenching rate constant
ΔH (*)	Enthalpy changes in the ground (excited) state
ΔG (*)	Free energy changes in the ground (excited) state
ΔS	Entropy change
N_A	Avogadro's number
ν	Frequency
h	Planck's constant
n	Refractive index
pK_a(*)	Ground(excited) state acidity constant
R	Universal gas constant
T	Temperature in Kelvin
K_a(*)	Ground (excited) state equilibrium dissociation constant
RO^{-*}	Excited-state anionic photoacid

E_T^N	Solvent polarity parameter
Δf	Field factor
ROH*	Excited-state neutral photoacid
λ	Wavelength
λ_{abs}^{max}	Maximum wavelength in the absorption spectrum
$\lambda_{abs}, \lambda_{em}$	Absorption and emission wavelength
t	Time
τ	Excited state fluorescence lifetime in presence of quencher
Φ_F	Fluorescence quantum yield
pK_a	Acid dissociation constant
^1L_b, ^1L_a	The first two electronic transitions of phenol and phenolate ion
S_0	Electronic ground singlet state
S_1	The first excited singlet state
T_1	The first excited triplet state
α	Hydrogen bond donating power of the solvent
β	Hydrogen bond accepting power of the solvent
π^*	Solvent polarity/polarizability effect
f_i	Relative integrated fluorescence Intensity
a_i	Amplitude
k_p, k_p^*	The ground and excited state protonation rate constants

List of Abbreviations

Abbreviation	Scientific Name
1NO	1-naphthol
1NO4S	1-naphthol-4-sulfonic acid, Na salt
2NO	2-naphthol
5CN2NO	5-cyano-2-naphthol
DMSO	Dimethylsulfoxide
ESPT	Excited-state proton transfer
$ESI_{er}PT$	Excited-state intermolecular proton transfer
PT	Proton transfer
SA	Solvent's acidity
SB	Solvent's basicity
SdP	Solvent dipolarity
SP	Solvent polarizability
DI	Dispersion and induction interaction
ES	Electrostatic interaction
KT	Kamlet-Taft
S	Slope
LSERs	Linear solvation energy relationships
EtOH	Ethanol

EWG	Electron withdrawing group
FLT	Fluorescence lifetime
HOMO	Highest occupied molecular orbital
HPLC	High-performance liquid chromatography
ICT	Intramolecular charge transfer
IRF	Instrument response function
MeOH	Methanol
MLCs	Metal-ligand complexes
NMR	Nuclear magnetic resonance
LED	Light emitting diode
LUMO	Lowest unoccupied molecular orbital
PTTS	Proton transfer to solvent
TCSPC	Time-correlated single photon counting
UV-vis	Ultraviolet-visible