

**Ain Shams University
Faculty of Science
Chemistry Department**



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

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Approval Sheet

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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_0	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^0	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
$\Delta H (*)$	Enthalpy changes in the ground (excited) state
$\Delta G (*)$	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
$\lambda_{\text{abs}}^{\text{max}}$	Maximum wavelength in the absorption spectrum
$\lambda_{\text{abs}}, \lambda_{\text{em}}$	Absorption and emission wavelength
t	Time
τ	Excited state fluorescence lifetime in presence of quencher
Φ_F	Fluorescence quantum yield
$\text{p}K_a$	Acid dissociation constant
${}^1\text{L}_b, {}^1\text{L}_a$	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