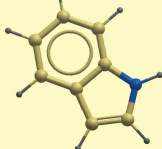
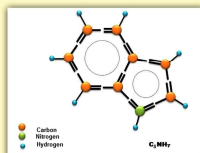
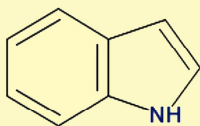


Introduction

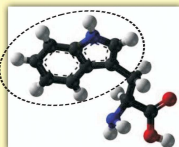
When a complex is formed the surface of the hydrophobic interior of the cyclodextrin and the hydrophobic exterior of the guest molecule exposed to hydrophilic solvent is decreased. It must be emphasized that the phenomenon of cyclodextrin inclusion compound formation is a complicated process and in reality there are many factors that play a role. Small molecules normally form 1:1 inclusion compounds. In such an inclusion compound, one cyclodextrin ring includes one guest.

Indole

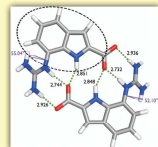
Indole is an aromatic heterocyclic compound with bicyclic structure consisting of a benzene ring fused to a five-membered nitrogen containing pyrrole.



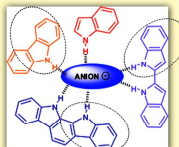
Organic compounds like tryptophan containing proteins, polymers and alkaloids consists of indole moiety.



Tryptophan



Polymers



As anion-binding agent

Indole is found in jasmynes, citrus plant, black locust plant and in coal tar. Indole is found in human cerebrospinal fluid and in human feces.



Jasmine



Citrus plant



Vinca minor



Black locust plant



Picalima Nitida



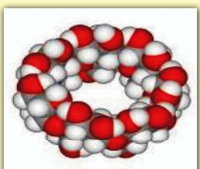
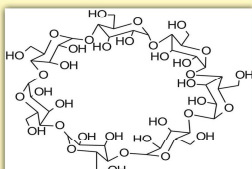
Coal tar

Indole and its derivatives are medicinally important compounds that possess a wide range of chemical, biological and pharmacological properties such as anti-depressive, anti-inflammatory, anti-bacterial, antimicrobial and anti-tuberculostatic.

Beta-Cyclodextrin

Cyclodextrins (CDs) are cyclic oligosaccharides obtained from enzymatic hydrolysis of starch

β -cyclodextrin is most abundant natural oligomers and corresponds to the association of seven glucose units with cavity, which exhibits a hydrophobic character whereas the exterior is strongly hydrophilic.



Methods



UV Spectroscopy



Cyclic Voltammetry



FTIR Spectroscopy



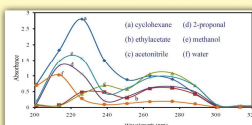
Powder XRD



Scanning Electron Microscope

Molecular Modeling Studies : PatchDock server and CycloPredict server.

Results and Discussion : Effect of solvents



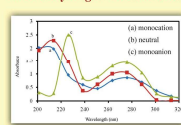
Absorption spectra of Indole in selected solvents at 303 K; concentration of Indole 1×10^{-4} M

The ϵ_{max} of SW band is high. These results imply that the SW band is attributed to the (π, π^*) transition of the benzene ring of the indole, whereas the LW band can be attributed to moiety of indole molecule

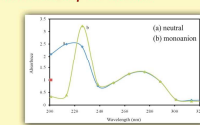
Solvatochromic shifts of indole reveals that the absorption maxima are red shifted from cyclohexane to 2-propanol but blue shifted in methanol and water.

The red shift observed in the absorption spectra moving from cyclohexane to acetonitrile is due to the dispersive interactions and the most proton accepting nature of acetonitrile.

Effect of hydrogen ion concentration with & without β -CD medium



Absorption spectra of different protonic species of Indole at 303 K; concentration of Indole 1×10^{-4} M



Absorption spectra of different protonic species of Indole at 303 K in b-CD medium

The pKa value for monoanion-neutral equilibrium of indole in β -CD medium differs appreciably than aqueous medium and this confirms the encapsulation of indole molecule in the β -CD cavity.

Various prototropic maxima (absorption spectra) and pKa values of Indole in with and without β -CD medium

Species	With β -Cyclodextrin		Without β -Cyclodextrin	
	$\lambda_{abs}(nm)$	pKa	$\lambda_{abs}(nm)$	pKa
Monoanion	-	-	270.0	-1.85
	271.0	-0.26	270.0	-1.38
Neutral	218.0	11	218.0	14.37
	271.0	12.0	271.1	14.81
Monoanion	223.0	-	227.0	-

HOST-GUEST INTERACTION OF INDOLE : β -CYCLODEXTRIN INCLUSION COMPLEX*

K. Sivakumar and M. Parameswari

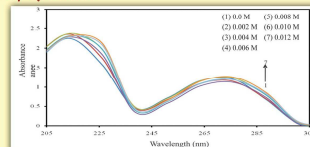
Department of Chemistry

Sri Chandrasekharendra Saraswathi Visva Mahavidyalaya University

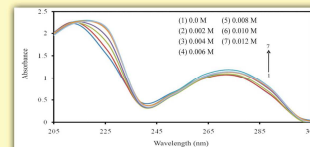
Enathur, Kanchipuram – 631 561, Tamil Nadu, India

Email: sivakumar.k@kanchiuniv.ac.in, chemparamu@gmail.com

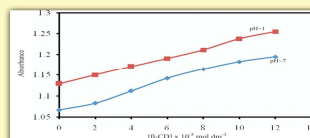
Effect of β -Cyclodextrin



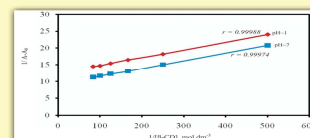
The absorption spectra of Indole (pH-1) in different β -CD concentrations



The absorption spectra of Indole (pH-7) in different β -CD concentrations



The Absorption intensity of Indole changes at 270nm with different β -CD concentrations in pH-1 and pH-7

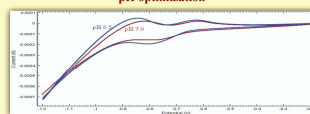


Benesi-Hildebrand plot of $1/A-A_0$ vs. $1/[\beta\text{-CD}]$ for Indole in pH-1 and pH-7 solution

The binding constant 'K' and stoichiometric ratios of the inclusion complex of indole can be determined according to the Benesi-Hildebrand relation assuming the formation of a 1:1 host-guest complex.

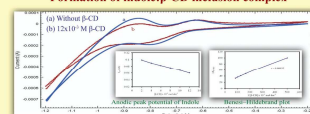
The electrochemistry of inclusion process

pH optimization

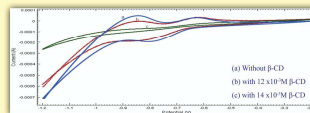


CVs of Indole 1×10^{-3} M at Pt electrode in phosphate buffer at pH 6.5 and pH 7; Scan rate 50 mVs⁻¹.

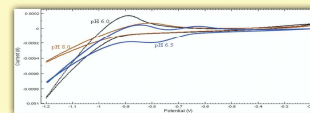
Formation of indole: β -CD inclusion complex



CVs of Indole: β -CD in pH 6.5 buffer solution; Scan rate: 50 mVs⁻¹, concentration of Indole: 1×10^{-3} M.



CVs of Indole in pH 6.5 buffer solution with scan rate: 50 mVs⁻¹, concentration of Indole: 1×10^{-3} M.

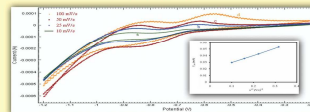


CVs of Indole (1×10^{-3} M) in phosphate buffer; Scan rate 50 mVs⁻¹.

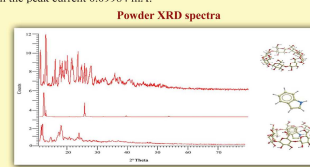
On increasing the β -CD concentration to 14×10^{-3} M, the oxidation peak current decreases drastically with the disappearance of oxidation and reduction peaks. This behavior has been attributed to the enhanced dissolution of indole molecule through the hydrophobic interaction between indole and β -CD.

The reduction peak (redox couple) disappears at pH above and below 6.5. This indicates that the protons are not involved in the oxidation process of indole at pH 6.5. Thus, at pH 6.5 the lone pair of electron gets oxidized at -863.04 mV with the peak current 0.09984 mA.

Effect of scan rate



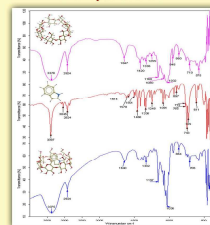
CVs of indole (1×10^{-3} M) with β -CD (12×10^{-3} M) in pH 6.5 buffer solution at different scan rates.



Powder XRD spectra

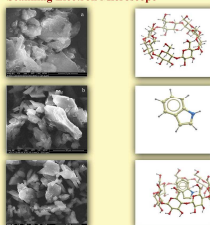
The linearity of the plot between $\log i_p$ and $\log \nu$ indicates that the electrochemical oxidation process of indole is controlled by the diffusion step over the range of scan rate studied

FTIR spectral studies



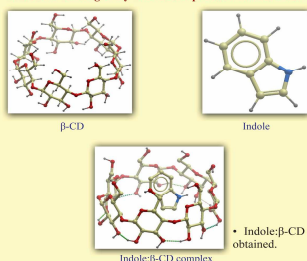
FTIR Spectra of (a) β -CD, (b) Indole, (c) Indole: β -CD solid complex in KBr.

Scanning Electron Microscope

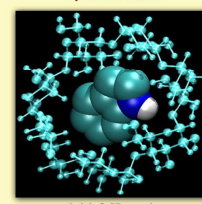


SEM pattern of (a) β -CD (b) indole (c) indole: β -CD solid complex

Molecular docking study of inclusion process : PatchDock server



CycloPredict server



The docking result of CycloPredict server is slightly differing from the results obtained through experimental methods and Patchdock server.

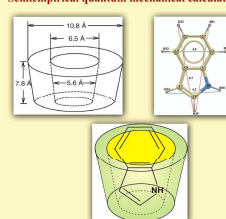
Conclusions

In summary, the inclusion complex with 1:1 molar ratio was formed between indole and β -CD.

References

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2. H. Kim et al., *J. Phys. Chem.*, 100 (1996) 15670.
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Semiempirical quantum mechanical calculations



Indole: β -CD 1:1 host guest mechanism