



Research Article

Preparation of Copper –3-Aminophenol–Cyclodextrin Nanomaterials and Study of 3-Aminophenol–Cyclodextrin Inclusion Complexes at Different pH Conditions

Narayanasamy Rajendiran^{1,*} , Ayyadurai Mani² , Palanichamy Ramasamy³

¹Department of Chemistry, Annamalai University, Annamalai Nagar, India

²Center for Advanced Energy Materials, SRM TRP Engineering College, Tiruchy, India

³Molecular Biophysics Unit, Indian Institute of Science, Bangalore, India

Abstract

The spectral behavior of 3-aminophenol (3AP) with α -cyclodextrin (α -CD), β -cyclodextrin (β -CD) in pH ~2, pH ~7, pH ~11 and copper nano was investigated using UV–visible absorption, steady-state and time-resolved fluorescence, PM3 calculations, SEM, DSC, FTIR, XRD, and ¹H NMR techniques. 3AP exhibited a single emission band at the same wavelength in α -CD at pH ~2 and pH ~7, whereas dual emission was observed at pH ~11. Across all solvents, the absorption and emission maxima of 3AP resembled those of 3-anisidine. In β -CD, the emission intensity at pH ~7 and pH ~11 decreased at the shorter-wavelength (normal emission) band and increased at the longer-wavelength band, suggesting the presence of an intramolecular charge-transfer (ICT) process in 3AP. The lifetimes of the inclusion complexes were longer than that of the free 2AP molecule. The geometrical restriction of the α -CD cavity likely limits the free rotation of the amino and hydroxyl groups, thereby enhancing the intensity of the IPT emission. The calculated HOMO–LUMO energy gap, total energy, free energy, enthalpy, entropy, dipole moment, and zero-point vibrational energy of the CD: 3AP complex differed significantly from those of the isolated 2AP, α -CD and β -CD molecules, and both the vertical and horizontal bond lengths between the amino and hydroxy groups are smaller than the β -CD cavity size confirming the formation of an inclusion complex. The lifetimes of the 3AP–CD inclusion complexes were longer than that of free 3AP. SEM-EDX analysis confirmed the presence of 48% carbon, 47.3% oxygen, and 3.3% copper in the nanomaterials. In DSC, XRD, and FTIR analyses, new peaks appeared along with a substantial reduction in the intensity of characteristic bands for the nano Cu-3AP-CD complex, indicating successful complex formation and structural modification.

Keywords

3-Aminophenol, Copper Nano, Cyclodextrin, Inclusion Complex, Nanomaterials

1. Introduction

Cyclodextrins (CDs) are an important class of supramolecular assemblies that have attracted increasing attention over

the years because of their potential applications as molecular devices and functional materials [1-15]. CDs are chemically

*Correspondence: Narayanasamy Rajendiran (drrajendiran1967@gmail.com)

Received: 11 March 2026; Accepted: 23 March 2026; Published: 2 April 2026



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stable molecules that can be modified either fully or regioselectively, producing analogues with enhanced solubility and versatile complexation properties. Through simple inclusion complexation between CDs (receptors) and drug molecules (substrates), numerous nanometer-sized supramolecular aggregates have been fabricated, demonstrating significant promise for use as molecular machines, molecular devices, and functional materials [11-15]. CDs form inclusion complexes with a wide range of chemicals, including fungicides, insecticides, herbicides, pheromones, repellents, and growth regulators. In the pharmaceutical industry, CDs are mainly employed as: (i) complexing agents to enhance the aqueous solubility of poorly soluble drugs, (ii) stabilizers to improve drug bioavailability and shelf life, and (iii) agents that reduce the volatility of sensitive drug molecules.

In this context, the present study aims to investigate: (i) the absorption and fluorescence spectral shifts and the first excited singlet-state lifetimes of 3-aminophenol (3AP) in α -CD, β -CD, and solvents of varying polarity and pH, (ii) the proton-transfer behavior of 3AP in aqueous, α -CD, and β -CD media, (iii) the structures and geometries of the resulting inclusion complexes using PM3 molecular modeling, and (iv) the doping effect of the 3AP: CD system on Ag nanomaterials using DSC, FTIR, ^1H NMR, and SEM analyses [16-20].

2. Materials and Methods

2.1. Preparation of CD Solution

The concentration of the 3AP stock solution was 2×10^{-2} mol/dm³. Aliquots of 0.1 or 0.2 mL of this stock solution were transferred into 10 mL volumetric flasks. Varying concentrations of α -CD or β -CD ($0.2, 0.4, 0.6, 0.8$, and 1.0×10^{-2} mol/dm³) were added, and the mixtures were diluted to 10 mL with triply distilled water and shaken thoroughly. The final concentration of 3AP in all flasks was 4×10^{-4} mol/dm³. All experiments were performed at room temperature (298 K).

2.2. Synthesis of Cu: 3AP: CD Nanomaterials

A 100 mL solution of CuSO_4 (1×10^{-3} mol/dm³) placed in a round-bottom flask was reduced by the dropwise addition of 1% sodium borohydride while stirring vigorously on a hot plate equipped with a magnetic stirrer. During the reduction process, the solution color changed from pale blue to reddish brown. Subsequently, 5 mL of 1% trisodium citrate was added dropwise to act as a stabilizer.

For the preparation of the inclusion nanomaterials, CD (1 mmol) was dissolved in 40 mL of distilled water, and 3AP (1 mmol), dissolved in 10 mL of ethanol, was added slowly to the CD solution. The mixture was stirred at 50 °C for 2 hours. The copper nanoparticle solution was then added to this mixture and stirred for an additional 2 hours at 40–50 °C. The resulting product was freeze-dried using a mini-lyophilizer at –80 °C to obtain a solid powder. The Cu-3AP-CD nanomaterial

was washed with small amounts of ethanol and water to remove uncomplexed drug, copper, and CD. The purified precipitate was dried under vacuum at room temperature and stored in an airtight container. The resulting Cu: 3AP: CD powder samples were used for further analyses [16-20].

3. Results and Discussion

3.1. Effect of pH on 3AP with α -CD and β -CD

Table 1, Figure 1, and Figure 2 present the absorption and emission maxima of 3AP (2×10^{-4} mol/dm³) in varying concentrations of α -CD and β -CD at pH ~3, pH ~7, and pH ~11. To compare the inclusion behavior of the neutral and monocationic species of 3AP with α -CD and β -CD, different pH conditions were employed. The spectral maxima of 3AP in CD-free aqueous solutions appear at the following wavelengths: pH ~3: $\lambda_{\text{abs}} \approx 272, 212$ nm; $\lambda_{\text{flu}} \approx 300$ nm; pH ~7: $\lambda_{\text{abs}} \approx 283, 232, 210$ nm; $\lambda_{\text{flu}} \approx 337$ nm; pH ~11: $\lambda_{\text{abs}} \approx 286, 216$ nm; $\lambda_{\text{flu}} \approx 338$ nm. These results indicate that neutral 3AP is predominant at pH ~7 and pH ~11, whereas the blue-shifted spectra at pH ~3 correspond to the monocationic form [21-29] and the monoanion exist at pH ~11 [30-37]. The emission maximum at 337 nm in pH ~7 resembles the spectra observed in non-aqueous solvents, validating that the molecular form of 3AP is predominant (Table 1).

In both α -CD and β -CD media, the absorption and emission features of 3AP at pH ~3 differ considerably from those at pH ~7 and pH ~11. No significant absorption shifts were observed with α -CD at any pH. For β -CD, no prominent absorption changes were noted at pH ~3 or pH ~11, whereas at pH ~7 the absorption maximum blue shifted from 283 to 273 nm [21-29]. In both CDs, the absorbance increased with CD concentration at all pH values. For α -CD, increasing concentrations enhanced the single emission maximum at 337 nm at pH ~3 and pH ~7, while dual emission appeared at pH ~11. At pH ~11, the shorter-wavelength (337 nm) intensity decreased while the longer-wavelength (430 nm) intensity increased. β -CD induced more pronounced effects: increasing β -CD concentration decreased emission intensity at all pH values. A single emission band was observed at pH ~3, whereas dual emission appeared at pH ~7 and pH ~11. In β -CD at pH ~7 and pH ~11, the short-wavelength (SW, normal emission) intensity decreased while the long-wavelength (LW, ICT) intensity increased. At pH ~11, the SW band exhibited a red shift with increasing β -CD, while the LW band remained unchanged.

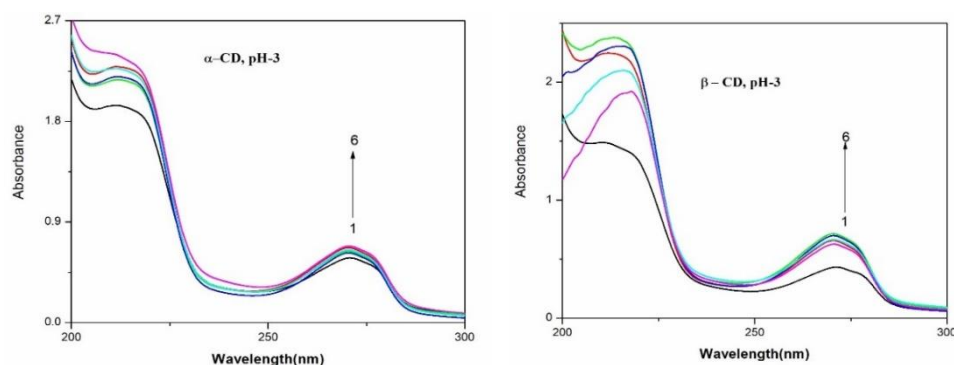
The changes in absorption and emission spectra in the presence of CDs (α and β) confirm the encapsulation of 3AP within the CD cavity and the formation of 1: 1 inclusion complex [21-37]. The presence of isosbestic points further supports a clean 1: 1 equilibrium, although the orientation of 3AP inside the cavity may vary at different pH values and CD concentrations. Binding constants (K) and ΔG values were calculated using Benesi-Hildebrand plots ($1/(A - A_0)$ vs $1/[\text{CD}]$)

and $1/(I - I_0) \text{ vs } 1/[CD]$), revealing linear relationships consistent with 1: 1 complex formation. The negative ΔG values (Table 1) indicate that the inclusion processes are spontaneous and exothermic at 303 K. At pH ~7 in β -CD, the observed blue shift suggests protonation of the amino group. These findings imply that in CD-free solutions structure I is favored, whereas in CD solutions structure II becomes more stable, explaining the pH-dependent emission behavior. The spectral variations

across different pH values suggest that hydrogen bonding interactions play an important role in inclusion complexation. At higher CD concentrations, the distinct changes in spectral shape indicate the formation of different types of inclusion complexes in α -CD and β -CD. Given that hydrophobic interactions drive encapsulation, the aromatic ring of 3AP preferentially enters the nonpolar CD cavity while the $-NH_2$ group remains closer to the rim [21-37].

Table 1. Absorption and fluorescence maxima of 3-Aminophenol (3AP) with different α -CD and β -CD concentrations.

Concentration of CD $\times 10^{-3} \text{ mol/dm}^3$	pH -3.0				pH - 7				pH - 11			
	λ_{abs}	$\log \epsilon$	λ_{flu}	τ	λ_{abs}	$\log \epsilon$	λ_{flu}	τ	λ_{abs}	$\log \epsilon$	λ_{flu}	τ
3AP only (in water)	272 212	3.43	300	0.30	283 232 210	3.49	337	0.33	286 216	3.48	338	0.29
0.2 α -CD	271 212	3.46	300	0.39	282 231 210	3.50	337	0.40	286 219	3.53	338	0.40
1.0 α -CD	270 212	3.51	300	0.48	282 230 210	3.58	336	0.54	289 221	3.58	339 431	0.51 0.19
0.2 β -CD	271 213	3.48	300	0.41	278 231 212	3.49	337	0.46	288 218	3.53	339 443	0.34
1.0 β -CD	272 217	3.54	306	0.50	273 218	3.63	337 430	0.54 0.22	289 227	3.64	355 443	0.55 0.25
Excitation wavelength (nm)			270				280				270	
K (1: 1) $\times 10^5 \text{ dm}^3/\text{mol}$	78		196		65		198		86		371	
$\Delta G \text{ (kcalmol}^{-1}\text{)}$	-10.97		-13.29		-10.51		- 13.32		-11.22		-14.90	
K (1: 1) $\times 10^5 \text{ dm}^3/\text{mol}$	86		285		104		204		115		486	
$\Delta G \text{ (kcalmol}^{-1}\text{)}$	-11.22		-14.24		-11.70		- 13.39		-11.95		-15.58	



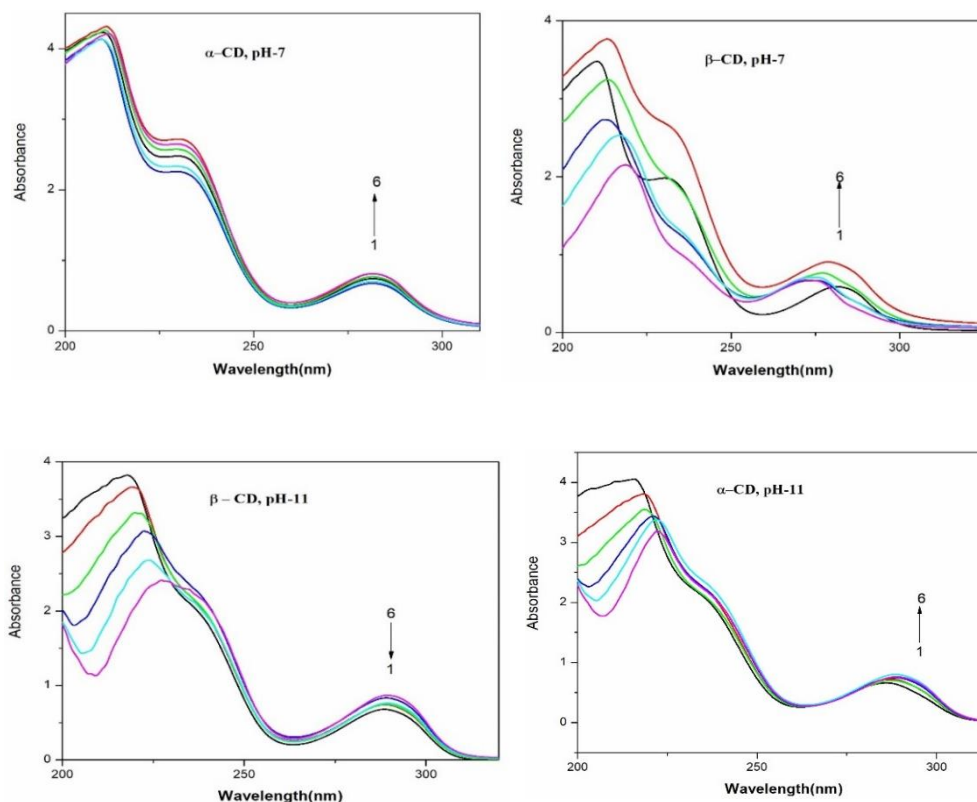
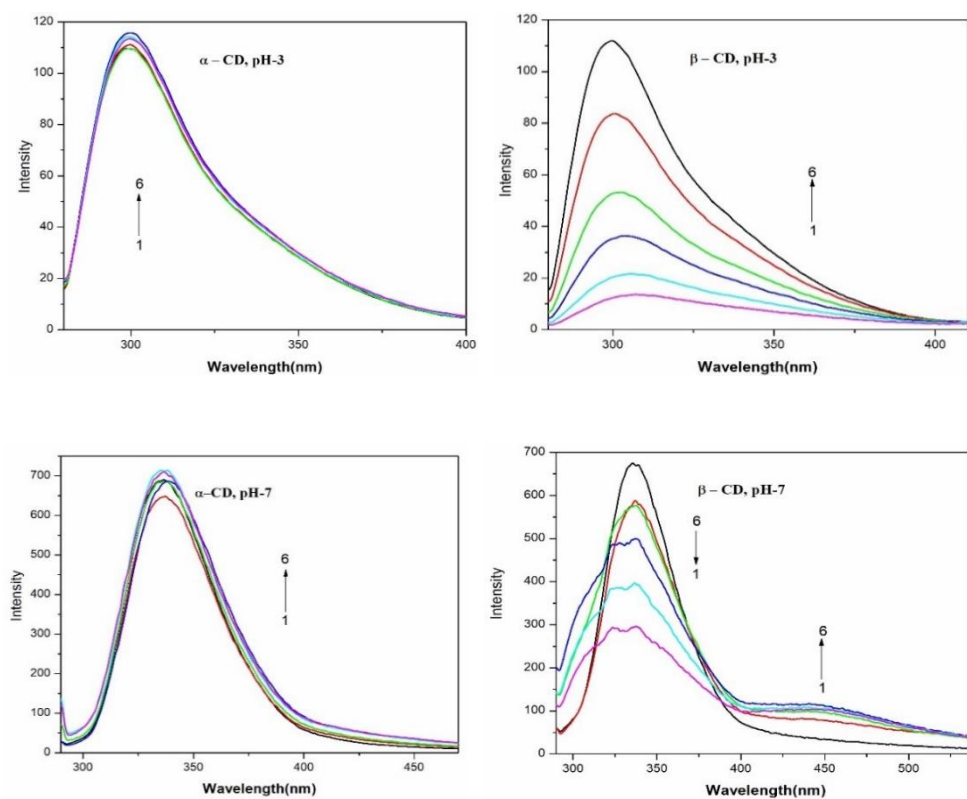


Figure 1. Absorbance spectra of 3AP in different α -CD and β -CD concentrations (mol/dm^3): (1) 0, (2) 0.002, (3) 0.004, (4) 0.006, (5) 0.008 and (6) 0.01.



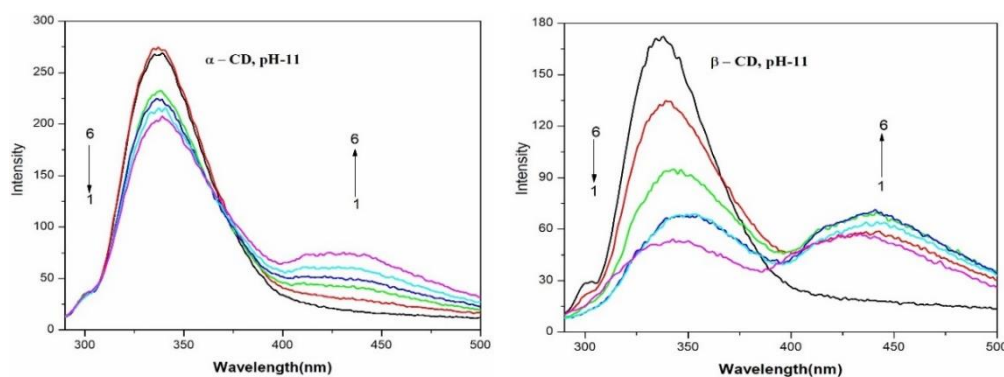


Figure 2. Fluorescence spectra of 3AP in different α -CD and β -CD concentrations (mol/dm^3): (1) 0, (2) 0.002, (3) 0.004, (4) 0.006, (5) 0.008 and (6) 0.01.

3.2. Intramolecular Charge Transfer Emission (ICT)

At pH ~ 7 , 3AP exhibits single emission in α -CD but dual emission in β -CD. At pH ~ 11 , dual emission becomes prominent at α -CD and β -CD concentrations above 4×10^{-3} M. ICT emission is stronger at pH ~ 11 than at pH ~ 7 , likely due to variations in polarity, viscosity, and cavity dimensions. To investigate the origin of dual emission, solvent-dependent spectral studies were performed. The absorption and emission maxima of 3AP in selected solvents were: (cyclohexane: $\lambda_{\text{abs}} \approx 286, 236$ nm; $\lambda_{\text{flu}} \approx 314$ nm, acetonitrile: $\lambda_{\text{abs}} \approx 289, 240$ nm; $\lambda_{\text{flu}} \approx 324$ nm, methanol: $\lambda_{\text{abs}} \approx 284, 235$ nm; $\lambda_{\text{flu}} \approx 327$ nm, water: $\lambda_{\text{abs}} \approx 282, 232$ nm; $\lambda_{\text{flu}} \approx 336$ nm. These values closely match those of 3-anisidine (3AS) [28], which shows single broad emission in all solvents, indicating that 3AP does not form ICT, exciplex, or excimer in homogeneous media.

Relative to aniline [29] and phenol [30–35], 3AP shows red-shifted absorption in all solvents, suggesting delocalization between the amino and hydroxy groups. In solvents and in α -CD, only a single emission band is observed, while β -CD induces dual emission at pH ~ 7 and pH ~ 11 . Dual emission consists of a SW band (337–356 nm) and a LW band (435–442 nm). Both bands red-shift with increasing β -CD, the SW shift being more pronounced.

Dual luminescence is characteristic of 4,4'-dimethylamino benzonitrile (DMABN) like systems [38–48], and previous studies support an ICT mechanism for 3AP in β -CD. The absence of ICT at pH ~ 2 is attributed to protonation of the amino group, which alters the encapsulation geometry. At pH ~ 7 and pH ~ 11 , the $-\text{NH}_2$ or $-\text{O}^-$ groups interact with the CD cavity. The nonpolar environment of the cavity restricts rotation, thereby suppressing ICT in α -CD but promoting it in β -CD. The higher number of hydroxyl groups at the CD rims creates an environment similar to polyhydroxy alcohols, facilitating hydrogen-bond-assisted ICT [21–37].

3.3. Excited Singlet State Lifetimes

The fluorescence lifetimes of 3AP and its CD inclusion

complexes were obtained from the decay curves (Table 1). The lifetimes of the inclusion complexes were longer than that of free 3AP. The lifetime of 3AP increased in the order: water $<$ α -CD $<$ β -CD. This trend suggests that the β -CD: 3AP inclusion complex is more stable than the α -CD complex, likely due to greater restriction of molecular vibrations in the excited state. The progressive increase in lifetime with increasing CD concentration further supports the encapsulation of 3AP within the CD cavity.

In aqueous solution, the monomer emission of 3AP exhibited a very short decay time, which was altered upon the addition of CDs. With CDs, the ICT emission decay profile became triexponential, accompanied by a marked increase in lifetime. Moreover, different ICT decay components appeared with increasing CD concentrations, indicating the formation of inclusion complexes. Notably, the rise time of the ICT emission—distinct from the fast decay of the normal emission—became longer as CD concentration increased, whereas no rise time was observed in water. These observations demonstrate that the ICT process in the CD: 3AP inclusion complex differs significantly from that in water. Overall, the results confirm that ICT formation is more favorable in CD solutions than in aqueous medium.

3.4. Molecular Modeling

The ground-state geometries of 3AP and the CDs were optimized using the PM3 method, and the corresponding thermodynamic parameters are listed in Table 2. Both α -CD and β -CD possess the same height (7.8 Å). The interior cavity diameter of α -CD ranges from 4.7 to 5.3 Å, while that of β -CD ranges from 6.0 to 6.5 Å. Their exterior diameters are 8.8 Å for α -CD and 10.8 Å for β -CD. Thus, both the interior and exterior cavity dimensions of α -CD are smaller than those of β -CD.

For 3AP, the vertical and horizontal distances between the $-\text{NH}_2$ and $-\text{OH}$ groups are 6.72 Å and 5.44 Å, respectively (Figure 3). These distances are both smaller than the β -CD cavity size, indicating that 3AP can readily fit inside the β -CD cavity. In contrast, while the vertical distance in 3AP is

smaller than the α -CD cavity, the horizontal distance exceeds the α -CD interior diameter. Therefore, the guest molecule cannot be fully accommodated within the α -CD cavity. These observations suggest that 3AP forms different types of inclusion

complexes with α -CD and β -CD. Optimization of the inclusion complex geometries further confirmed that the guest molecule is only partially inserted into the CD cavity.

Table 2. Thermodynamic parameters and HOMO-LUMO energy calculations for 3AP and its inclusion complexes by PM3 method.

Properties	3AP	α -CD	β -CD	3AP: α -CD	3AP: β -CD
E_{HOMO} (eV)	-8.55	-10.37	-10.35	-8.06	-8.18
E_{LUMO} (eV)	0.35	1.26	1.23	0.79	0.88
$E_{\text{HOMO}} - E_{\text{LUMO}}$ (eV)	-8.91	-11.63	-11.58	-8.85	-9.06
Dipole moment (D)	2.96	11.34	12.29	12.14	12.32
E^*	-25.79	-1247.62	-1457.63	-1361.34	-1535.61
ΔE^*				-187.94	-52.2
G^*	50.04	-676.37	-789.52	-586.12	-668.12
ΔG^*				-40.18	-50.62
H^*	74.52	-570.84	-667.55	-516.79	-610.84
ΔH				-20.47	-17.81
S^{**}	0.082	0.353	0.409	0.461	0.482
ΔS^{**}				0.026	-0.009
ZPE*	65.84	635.09	740.56	703.62	781.83
Mullikan charge	0.00	0.00	0.00	0.00	0.00

*kcal/mol; **kcal/mol-Kelvin; ZPE = Zero point vibration energy

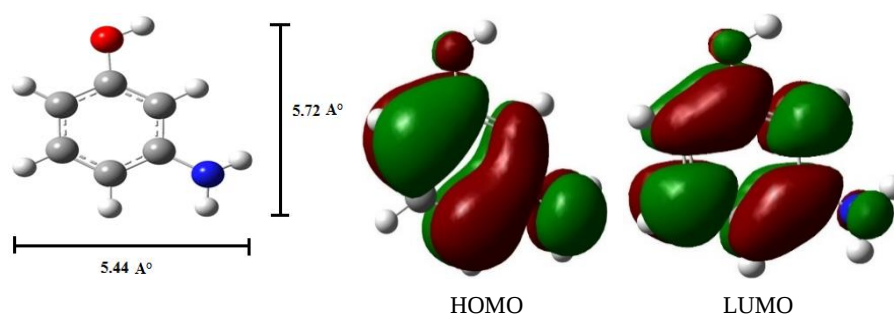


Figure 3. PM3 optimized structures of (a, b) 3AP (c, d) HOMO, LUMO of 3AP.

Significant changes in the HOMO–LUMO energies, free energy, enthalpy, entropy, dipole moment, and zero-point vibrational energy of the CD: 3AP complexes compared with isolated 3AP demonstrate the formation of inclusion complexes. The polarity of the CDs also changes upon guest entry into the cavity. The negative values of the energy, enthalpy, and Gibbs free energy changes indicate that the inclusion processes are both energetically and enthalpically favorable. Moreover, the binding energies (ΔE) of the complexes are higher than those of the isolated 3AP molecule, confirming

the enhanced stability of the inclusion complexes.

3.5. Inclusion Complex Nanomaterials Studies

3.5.1. Scanning Electron Microscope

The powdered forms of copper nanoparticles, 3AP, and the Cu: 3AP: α -CD and Cu: 3AP: β -CD nanomaterials were examined using SEM (Figure 4). The images clearly reveal that

copper nanoparticles appear as clustered particles, 3AP exhibits a microrod-like morphology, the Cu: 3AP: α -CD complex shows a stone-like structure, and the Cu: 3AP: β -CD complex displays a nanorod-shaped morphology. SEM-EDX analysis confirms the presence of 48% carbon, 47.3% oxygen, and 3.3% copper in the nanomaterials. The distinct morphologies of pure Cu nano, 3AP, and their inclusion complexes further support the successful formation of the Cu: 3AP: CD nanomaterials.

3.5.2. Differential Scanning Colorimeter

The DSC thermograms of α -CD, β -CD, 3AP, and their corresponding inclusion complexes were also evaluated. α -CD exhibits three endothermic peaks at 79.2 °C, 109.1 °C, and 137.5 °C, whereas β -CD shows a broad endothermic peak at 128.6 °C; these peaks correspond to the loss of crystalline water from the cyclodextrins. 3AP displays sharp thermal transitions at 120 °C and 164 °C, corresponding to its melting and boiling points. Broad endothermic features observed for α -CD, β -CD, and their complexes arise from water loss in the CD cavities. Notably, the DSC curves of the Cu-3AP-CD inclusion complexes do not show the characteristic peaks of pure

3AP and CDs. Instead, new thermal events appear at 274 °C for Cu: 3AP: α -CD and 291 °C for Cu: 3AP: β -CD, confirming the formation of new inclusion complexes.

3.5.3. Infrared Spectral Studies

In the isolated 3AP molecule (Figure 5), the N-H, O-H, and C-H stretching bands appear at 3361, 3296, and 3043 cm^{-1} , respectively. The N-H bending vibration and aromatic C=C stretching modes are observed at 1699, 1606, and 1509 cm^{-1} . The aromatic C-C, C-OH, and C-O stretching vibrations occur at 1468, 1180, and 1304 cm^{-1} , respectively. The C-O-C and C-N stretching frequencies are noted at 1259, 1180, and 1360 cm^{-1} . The out-of-plane O-H vibration appears at 696 and 690 cm^{-1} .

In the nanomaterials, the NH_2 and O-H stretching bands shift to 3230 and 2912 cm^{-1} , respectively, while the aromatic C=C and C-O stretching vibrations appear at 1608 and 1336 cm^{-1} . The aromatic ring deformation band is observed at 584 cm^{-1} . A significant reduction in intensity for the Cu: 3AP: CD nanocomplexes indicates strong interactions between 3AP and the copper nanoparticles.

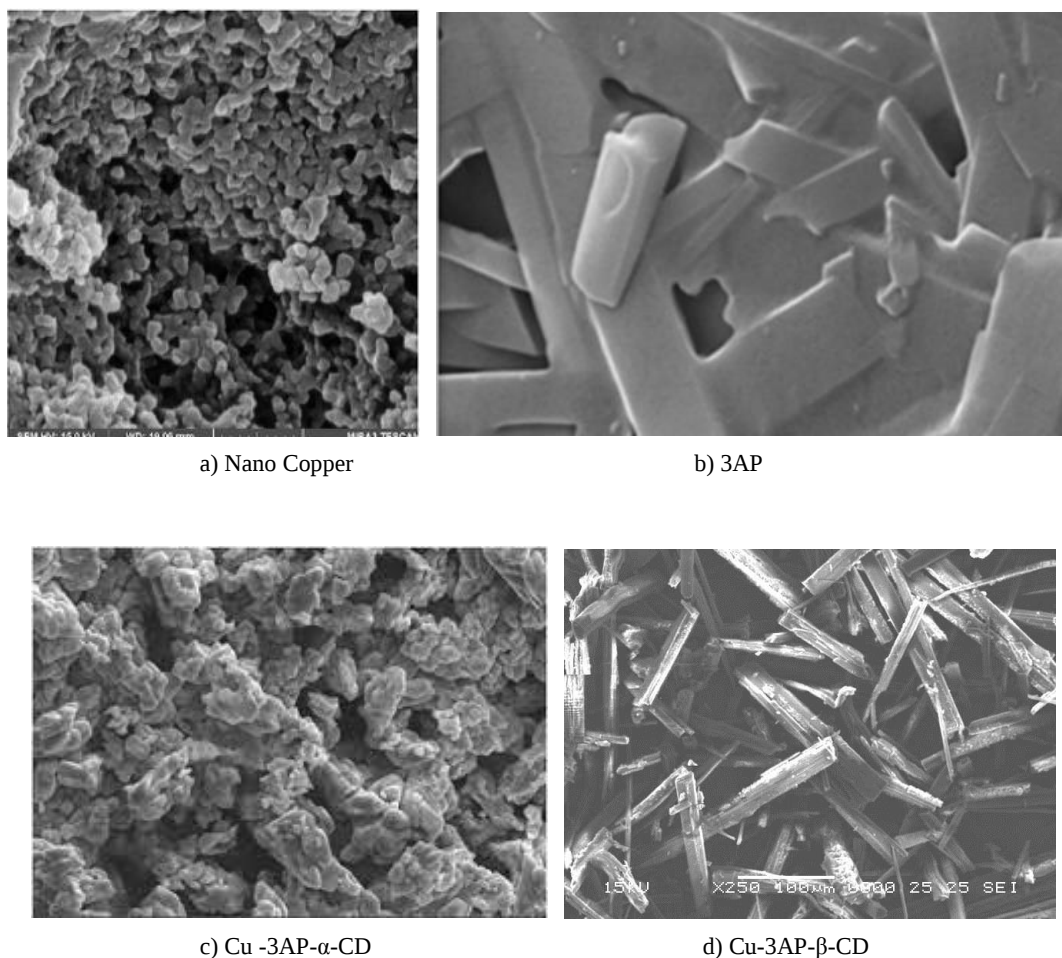


Figure 4. SEM images for a) Cu nano, b) 3AP, c) Cu: 3AP: α -CD and d) Cu: 3AP: β -CD.

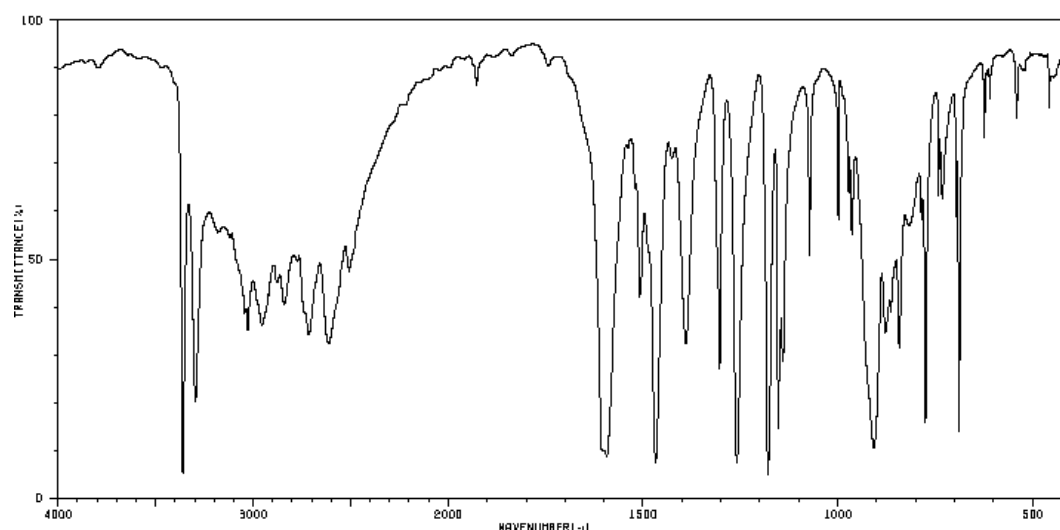


Figure 5. 12 FTIR spectra of 2AP.

3.5.4. XRD Spectral Studies

The crystalline nature of all nanoparticles was examined using XRD analysis. Pure copper nanoparticles exhibit prominent diffraction peaks at 43.31° , 50.44° , and 74.20° , characteristic of the face-centered cubic structure of metallic copper. The XRD pattern of α -CD shows crystalline reflections at approximately 11.94° , 14.11° , and 21.77° , while β -CD displays peaks at 11.49° and 17.58° ; the exact intensities may vary depending on sample preparation. 3AP crystallizes in an orthorhombic system, showing diffraction peaks at 8.23° , 8.73° , and 20.61° . The XRD pattern of the Cu/3AP: β -CD nanomaterial exhibits distinct peaks at 13.13° , 18.26° , 26.23° , 29.74° , 36.61° , 44.82° , and 75.78° . The changes in peak intensity and position relative to the pure components confirm the formation of new nanomaterials.

3.5.5. ^1H NMR Spectral Studies

^1H -NMR spectra of 3AP (Figure 6) and its inclusion complexes were recorded at 25°C in DMSO-d_6 (Table 3). NMR spectroscopy provides information on proton chemical shifts, host-guest interactions, signal broadening, and resolution changes. The proton resonances of cyclodextrins are well established and include six distinct types of protons. Among these, the H-3 and H-5 protons, located inside the CD cavity, experience chemical shift changes upon guest inclusion. In contrast, protons H-1, H-2, and H-4, situated on the exterior of the cavity, show only minor shifts.

Guest protons typically exhibit noticeable chemical shift variations when included within the CD cavity. In the presence of copper nanoparticles and CDs, the 3AP proton signals shift upfield, indicating interactions between 3AP, copper nanoparticles, and the cyclodextrin cavity. These observations confirm that all the 3AP protons are involved in interactions within the Cu: 3AP: CD nanomaterials.

Table 3. ^1H -NMR chemical shift values for the 3AP and Cu: 3AP: CD nanomaterials.

Protons	3AP (δ)	Cu: 3AP: α -CD	Cu: 3AP: β -CD
H _a -OH	8.83	5.73	5.75
H _b - Meta to OH	6.78	5.66	5.69
H _c - In between to OH and NH ₂	6.02	4.80	4.82
H _d - Ortho OH	6.01	4.46	4.49
H _e - Ortho to NH ₂	5.94	2.8	2.51
H _f -NH ₂	4.85	1.20	1.23

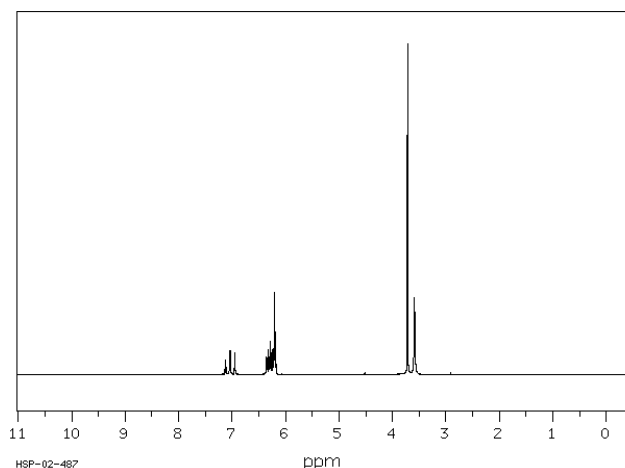


Figure 6. ^1H -NMR spectra of 3AP.

4. Conclusion

The spectral behaviour of 3-aminophenol (3AP) with α -CD and β -CD in solutions of pH $\sim$ 2, pH $\sim$ 7, and pH $\sim$ 11 was investigated using UV-visible spectroscopy, fluorescence and time-resolved fluorescence measurements, PM3 calculations, SEM, DSC, FTIR, XRD, and ^1H NMR techniques. In CD-free solutions, the emission maxima at pH $\sim$ 7 and pH $\sim$ 11 remain identical, whereas a different emission maximum is observed at pH $\sim$ 2. In the presence of α -CD or β -CD, no significant absorption shifts occur at pH $\sim$ 2 and pH $\sim$ 11; however, a blue shift is observed in β -CD at pH $\sim$ 7. In the excited state, increasing α -CD concentration leads to enhanced single-wavelength emission at pH $\sim$ 2 and pH $\sim$ 7, while dual emission appears at pH $\sim$ 11. Across all media, the absorption and emission maxima of 3AP resemble those of 3-anisidine. In β -CD at pH $\sim$ 7 and pH $\sim$ 11, the shorter-wavelength (normal) emission decreases, while the longer-wavelength emission increases, indicating the presence of an ICT process in 3AP. The lifetimes of the inclusion complexes are higher than that of free 3AP. SEM-EDX analysis confirms the presence of 48% carbon, 47.3% oxygen, and 3.3% copper in the nanomaterials. In DSC, XRD, and FTIR analyses, new peaks appear and a pronounced decrease in intensity is observed for the nano Cu-3AP-CD complexes, confirming structural and interactional changes upon complex formation.

Abbreviations

FTIR	Fourier Transform Infrared Spectroscopy
DTA	Differential Thermal Analysis
XRD	X-ray Diffraction
SEM	Scanning Electron Microscopy
HOMO	Highest Occupied Molecular Orbital
LUMO	Lowest Unoccupied Molecular Orbital
3AP	3-aminophenol
Ag NPs	Silver Nanoparticles
α -CD	Alpha Cyclodextrin

β -CD	Beta Cyclodextrin
PM3	Parametric Method 3
ΔE	Internal Energy Change
ΔH	Enthalpy Change
ΔG	Free Energy Change
ΔS	Entropy Change

Author Contributions

Narayanasamy Rajendiran: Methodology, Resources, Software, Supervision, Writing – original draft, Writing – review & editing

Ayyadurai Mani: Data curation, Formal Analysis, Investigation, Validation

Palanichamy Ramasamy: Data curation, Formal Analysis

Conflicts of Interest

The authors declare no conflict of interest.

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