

Research Article

Synthesis of Copper: 2-Anisidine: Cyclodextrin Nanomaterials and Characterization of 2-Anisidine–Cyclodextrin Inclusion Complexes at Various pH Conditions

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Abstract

Absorption, emission, time resolved fluorescence spectra and molecular modelling of 2-anisidine (2AS) with α -CD and β -CD in pH~2, pH~7 and pH~11 solutions were examined. Cu: 2AS: CD nanomaterials were investigated by SEM, DSC, FTIR, XRD and ¹H NMR techniques. The absorption and emission maxima and spectral shape of 2AS in all the pH solutions and solvents are different from each other. 2AS gave a single broad emission spectrum in all the solvents while dual emission noticed at pH~11. The lifetimes of the inclusion complexes were longer than that of the free 2AS molecule. The geometrical restriction of the α -CD cavity likely limits the free rotation of the amino and methoxy groups, thereby enhancing the emission intensity. The calculated HOMO–LUMO energy gap, total energy, free energy, enthalpy, entropy, dipole moment, and zero-point vibrational energy of the CD: 2AS complex differed significantly from those of the isolated 2AS, α -CD and β -CD molecules, and both the vertical and horizontal bond lengths between the amino and methoxy groups are smaller than the β -CD cavity size confirming the formation of an inclusion complex. In FTIR, most of the peaks are not appeared and a substantial decrease in intensity was noted in the Cu: 2AS: CD nano. The chemical shift value of 2AS protons are shifts to up field and down field and the peak intensities are very low in the nano copper with CD nanomaterials. SEM image of the nanomaterials are different from isolated 2AS molecule.

Keywords

2-Anisidine, Copper Nano, Cyclodextrin, Inclusion Complex, Nanomaterials

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1. Introduction

The design and fabrication of supramolecular nanostructures is a rapidly advancing field that continues to draw significant attention due to their inherent scientific importance and broad technological applications [1-5]. These nanostructures are widely explored for targeted drug or gene delivery, biochemical sensing, electronic and photonic materials, and nanoreactor systems [6-10]. Compared to constructing structures through step-by-step covalent synthesis, self-assembly offers a more efficient and environmentally friendly approach for generating supramolecular architectures. Spontaneous or externally induced self-assembly and chemical transformations of biological or organic building blocks (molecules, macromolecules, or supramolecular units) play a crucial role in achieving well-defined nanostructures and in precisely controlling supramolecular function at the molecular level [11-15].

From a medical research perspective, these systems are particularly important because of their potential in selective and targeted drug delivery. Achieving precise delivery to diseased cells remains a major challenge for chemists and biologists, as it requires ensuring that the drug remains protected throughout its transport and release. Supramolecular assemblies can offer such protective environments for drug molecules [16-20].

In light of these considerations, the present manuscript investigates: (i) the absorption and fluorescence spectral shifts and the first excited singlet-state lifetime of 2-anisidine (2-methoxyaniline, 2AS) in α -CD, β -CD, and solvents of varying polarity and pH; (ii) the proton-transfer behavior of 2AS in aqueous, α -CD, and β -CD media; (iii) the structures and geometries of the inclusion complexes using PM3 molecular modeling; and (iv) the doping effects of 2AS: CD on copper nanomaterials studied using DSC, FTIR, ^1H NMR, and SEM [21-25].

2. Materials and Methods

2.1. Preparation of CD Solution

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

2.2. Synthesis of Copper Nano and Cu: 2AS: 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 solution, under vigorous stirring on a

magnetic stirrer-hot plate. As the reaction proceeded, the solution color changed from pale blue to reddish brown. Subsequently, 5 mL of 1% trisodium citrate was added dropwise as a stabilizing agent.

Separately, CD (1 mmol) was dissolved in 40 mL of distilled water, and 2AS (1 mmol) dissolved in 10 mL of ethanol was slowly added to the CD solution. The mixture was stirred at 50 °C for 2 hours. The prepared copper nanoparticle solution was then added to this mixture and stirred for an additional 2 hours at 40–50 °C. The resulting solution was freeze-dried using a mini lyophilizer at –80 °C to obtain a powdered material. The Cu–2AS–CD nanomaterial was washed with small quantities of ethanol and water to remove unbound drug, copper, and CD. The product was then dried under vacuum at room temperature and stored in an airtight container. The resulting Cu: 2AS: CD powder samples were used for further characterization [21-25].

3. Result and Discussion

3.1. Effect of α -CD and β -CD and pH on 2-Anisidine

To compare the inclusion behavior of the neutral and monocationic forms of the guest molecule, the absorption and emission maxima of 2AS (2×10^{-4} mol/dm³) were recorded in various concentrations of α -CD and β -CD at pH $\approx 2, 7$, and 11 (Table 1, Figures 1 and 2). The spectral maxima of 2AS in aqueous solution are as follows: – pH ≈ 2 : $\lambda_{\text{abs}} \approx 269, 218$ nm; $\lambda_{\text{flu}} \approx 297$ nm; pH ≈ 7 : $\lambda_{\text{abs}} \approx 282, 231, 215$ nm; $\lambda_{\text{flu}} \approx 342$ nm; – pH ≈ 11 : $\lambda_{\text{abs}} \approx 282, 231$ nm; $\lambda_{\text{flu}} \approx 341$ nm. These results indicate that the neutral species predominates at pH ≈ 7 and pH ≈ 11 , whereas the blue-shifted absorption and emission bands at pH ≈ 2 confirm the presence of the monocationic form. At pH ≈ 7 , the emission maximum at 342 nm closely resembles that observed in non-aqueous solvents, supporting its assignment to the neutral molecular form of 2AS.

In water, α -CD, and β -CD media, the absorption and emission maxima of 2AS—and their spectral profiles vary with pH. In α -CD solutions, no appreciable absorption shifts were observed at any pH. In β -CD, the absorption maxima remain essentially unchanged at pH ≈ 2 and pH ≈ 11 , while a noticeable blue shift (from 282 to 272 nm) occurs at pH ≈ 7 . For α -CD, the absorbance of 2AS increases at the same wavelengths across all pH values. In contrast, in β -CD, the absorbance increases at pH ≈ 2 and pH ≈ 11 , but at pH ≈ 7 it decreases, accompanied by the observed blue shift.

In both α -CD and β -CD solutions, the emission maxima of 2AS vary across the different pH conditions (Figure 2). In α -CD, a single emission band is observed at pH ≈ 2 and pH ≈ 7 , whereas in β -CD, a single emission appears only at pH ≈ 2 ,

with dual emission emerging at $\text{pH} \approx 7$. At $\text{pH} \approx 11$, dual emission bands are present in both CD systems. At $\text{pH} \approx 2$, the emission maximum of 2AS in α -CD occurs at 297 nm, while at $\text{pH} \approx 7$ and $\text{pH} \approx 11$, the maxima appear at 340 nm and at 300, 341, and 440 nm, respectively. As the concentration of α -CD increases, the emission intensity increases at the same wavelengths—297 nm for $\text{pH} \approx 2$ and 340 nm for $\text{pH} \approx 7$. At $\text{pH} \approx 11$, dual emission is observed, and the intensities of both the short-wavelength (SW) and long-wavelength (LW) bands increase consistently at 341 and 440 nm, respectively.

In β -CD solutions, a single emission band is observed at pH

≈ 2 , while dual emission bands appear at $\text{pH} \approx 7$ and $\text{pH} \approx 11$. As the β -CD concentration increases, the emission intensity at $\text{pH} \approx 2$ decreases, accompanied by a red shift from 296 to 306 nm. At $\text{pH} \approx 7$, dual emission occurs: the short-wavelength (SW) band shows increased intensity along with a blue shift (296 to 306 nm), whereas the long-wavelength (LW) band increases in intensity without any shift, remaining at 440 nm. At $\text{pH} \approx 11$, the SW band intensity decreases with a red shift from 342 to 354 nm, while the LW band intensity increases at the unchanged wavelength of 440 nm.

Table 1. Absorption and fluorescence maxima of 2-Anisidine (2AS) with different α -CD and β -CD concentrations.

Concentration of α -CD $\times 10^{-3} \text{ mol/dm}^3$	pH - 2.0				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
2AS only (without CD)	269 215	2.38	297	0.59	282 231	3.53	342	0.61	282 231	3.41	341 300	- 0.54
0.002 mol/dm ³ α -CD	269 215	3.43	295	0.65	282 232	3.54	340	0.68	282 232	3.41	438 344 300	0.67 0.14
0.01 mol/dm ³ α -CD	269 215	3.41	296	0.80	283 233	3.59	340	0.82	283 231	3.40	438 342	0.82 0.24
0.002 mol/dm ³ β -CD	268 215	3.41	297	0.68	279 232	3.45	440 306	0.76 0.14	282 233	3.41	440 344	0.70 0.16
0.01 mol/dm ³ β -CD	269 216	3.47	305	0.87	273 214	3.36	440 306	0.86 0.24	283 232	3.47	440 354	0.89 0.26
α -CD- K (1: 1) $\times 10^5$ dm ³ /mol	89		278		62		229		88		124	
β -CD- K (1: 1) $\times 10^5$ dm ³ /mol	140		388		133		597		94		357	
α -CD- ΔG (kJmol ⁻¹)	-47.28		-59.41		-43.51		-57.32		-47.28		-48.53	
β -CD- ΔG (kJmol ⁻¹)	-52.3		-63.18		-51.46		-67.36		-48.12		-61.92	
Excitation wavelength (nm)			260				280				270	

In the excited state, the emission intensity of 2AS increases with rising α -CD concentration in all pH conditions. In contrast, with β -CD, the emission intensity decreases at $\text{pH} \approx 2$ and $\text{pH} \approx 11$ but increases at $\text{pH} \approx 7$. In CD-free aqueous solutions at $\text{pH} \approx 7$ and $\text{pH} \approx 11$, the longer-wavelength (LW) emission is very weak; however, it becomes increasingly prominent as the CD concentration increases, though it is absent in α -CD solutions at $\text{pH} \approx 7$. The observed variations in absorbance and emission upon addition of α -CD or β -CD indicate encapsulation of 2AS within the CD cavity [26-35], confirming the for-

mation of 2AS: CD inclusion complexes. At higher CD concentrations, changes in spectral maxima and band shapes in $\text{pH} \approx 2$, $\text{pH} \approx 7$, and $\text{pH} \approx 11$ suggest the formation of different types of inclusion complexes.

Across all pH conditions, the presence of an isosbestic point in the absorption spectra supports the formation of a 1: 1 inclusion complex, although the guest orientation within the CD cavity may differ [26-35]. Binding constants (K), obtained from Benesi-Hildebrand plots ($1/(A - A_0)$ vs $1/[\text{CD}]$ and $1/(I - I_0)$ vs $1/[\text{CD}]$), confirm a 1: 1 stoichiometry for the 2AS:

CD complex. The negative ΔG values indicate that the inclusion is spontaneous and exothermic (Table 1). At elevated α -CD and β -CD concentrations, the emission maxima and spectral profiles of 2AS vary significantly, further supporting the formation of different inclusion modes [26-35].

3.2. Intramolecular Charge Transfer (ICT) Emission

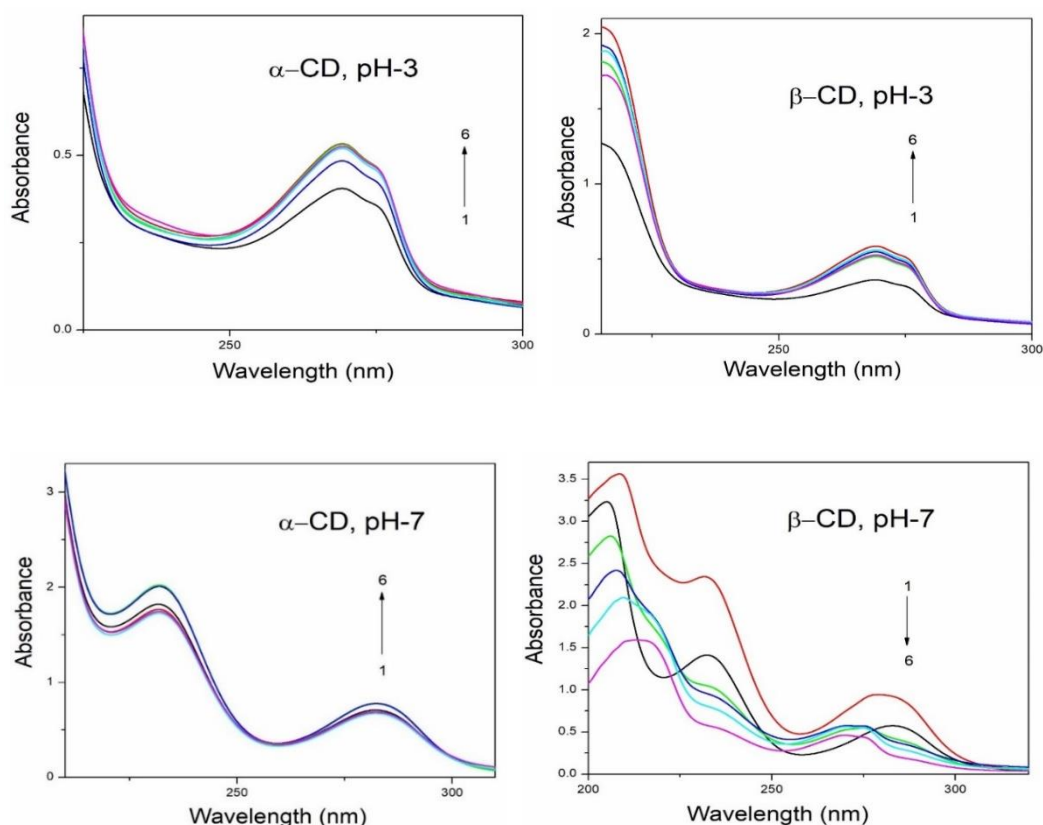
The 2AS/CD system displays a single emission band in water, pH ~3, and pH ~7, but exhibits dual emission at pH ~11. Above 4×10^{-3} mol/dm³ CD concentrations, a distinct dual-emission pattern characteristic of intramolecular charge transfer (ICT) becomes evident. Solvent-induced spectral shifts were examined to validate this dual emission. The absorption and emission maxima of 2AS in various solvents are as follows: cyclohexane ($\lambda_{\text{abs}} \approx 288, 238$ nm; $\lambda_{\text{flu}} \approx 321$ nm), acetonitrile ($\lambda_{\text{abs}} \approx 289, 240$ nm; $\lambda_{\text{flu}} \approx 331$ nm), methanol ($\lambda_{\text{abs}} \approx 285, 232$ nm; $\lambda_{\text{flu}} \approx 337$ nm), and water ($\lambda_{\text{abs}} \approx 282, 232$ nm; $\lambda_{\text{flu}} \approx 342$ nm). These values closely resemble the spectra of 2-aminophenol (2AP) [36], indicating similar photophysical behavior.

In all solvents, 2AS shows a single emission band, whereas dual emission arises only in α -CD and β -CD at pH 11. The absence of LW emission in solution suggests that ICT, exciplex, or excimer formation does not occur in the absence of CD. Slightly lower absorption and emission maxima for 2AS compared to 2AP imply weaker delocalization between the amino and methoxy groups. The dual emission consists of a

short-wavelength (SW, 340–355 nm) and a long-wavelength (LW, ~440 nm) band, with the LW intensity increasing at higher CD concentrations. Inside the α -CD cavity, the restricted polarity and reduced conformational freedom suppress both SW and LW emissions but enhance the normal/ICT band. At pH ~2, the protonated amino group is unlikely to enter the CD cavity, allowing free rotation of the amino and methoxy groups and preventing ICT formation. At pH ~11, identical emission maxima and spectral profiles in α -CD and β -CD suggest the occurrence of ICT emission [37-40].

3.3. Excited Singlet-State Lifetimes

Fluorescence lifetimes of 2AS and its α -CD complexes in aqueous and CD media were obtained from decay profiles (Table 1). In aqueous solution, 2AS exhibits biexponential decay at pH 2 and pH 7, and triexponential decay at pH 11. In β -CD, biexponential decay occurs at pH 2, whereas triexponential decay is observed at pH 7 and pH 11. The longer lifetimes in the inclusion complexes compared to free 2AS result from restricted vibrational relaxation within the CD cavity. The systematic increase in lifetime with increasing CD concentration reflects enhanced encapsulation of 2AS. The multiexponential decay indicates the coexistence of two emissive species whose dynamics compete with the conformational relaxation necessary for ICT formation. The slow component corresponds to ICT emission, suggesting rapid equilibrium between the locally excited (LE) and ICT states in water, which is shifted upon complexation with β -CD.



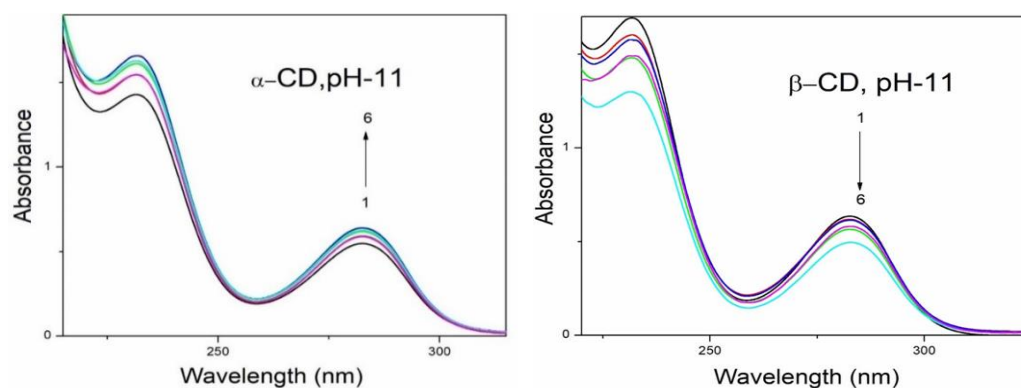


Figure 1. Absorption spectra of 2AS in different α -CD and β -CD concentrations (mol/dm^3): (1) 0, (2) 0.002, (3) 0.004, (4) 0.006, (5) 0.008 and (6) 0.01.

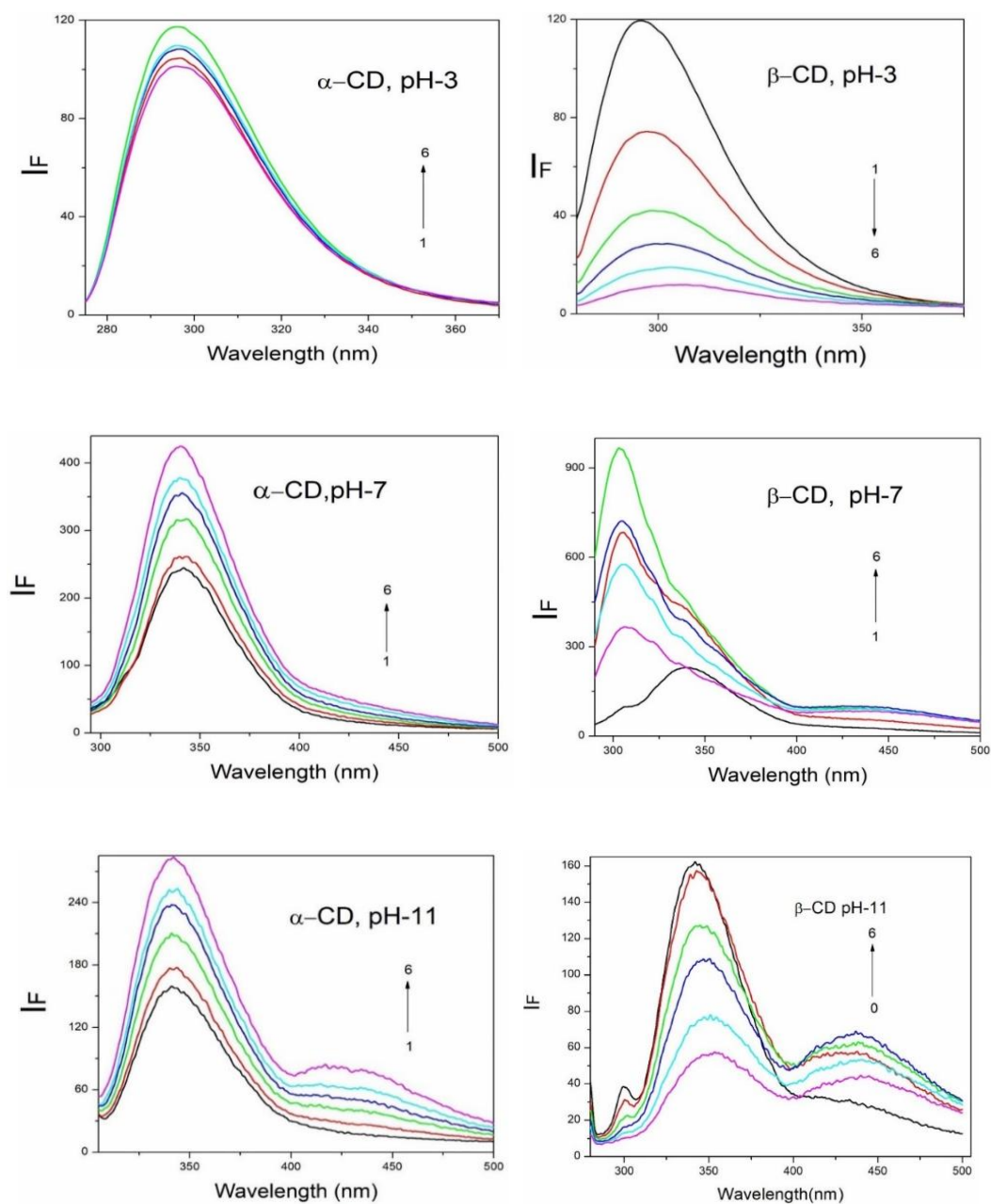


Figure 2. Fluorescence spectra of 2AS in different α -CD and β -CD concentrations (mol/dm^3): (1) 0, (2) 0.002, (3) 0.004, (4) 0.006, (5) 0.008 and (6) 0.01.

3.4. Molecular Modeling

Geometry optimizations of 2AS, CDs, and the inclusion complexes were carried out using the PM3 method (Figure 3). HOMO–LUMO energies, thermodynamic parameters (energy, enthalpy, entropy, Gibbs energy), dipole moments, zero-point energies, and Mulliken charges are summarized in Table 2. The height of α -CD and β -CD is 7.8 Å, with internal cavity diameters of 4.7–5.3 Å and 6.0–6.5 Å, respectively, and external diameters of 8.8 Å and 10.8 Å. In 2AS, the vertical and horizontal distances between the ring hydrogen and the OCH₃ group are 5.85 Å and 6.48 Å, respectively (Figure 3). The vertical distance fits within both CD cavities, but the larger horizontal distance

exceeds the CD diameters, implying partial rather than complete inclusion. This supports the formation of multiple inclusion modes in α -CD and β -CD. The optimized geometries show that 2AS undergoes slight structural adjustments—especially in dihedral angles—to adopt a stable conformation within the CDs.

The binding energy (ΔE), ΔG , and ΔH values for the 2AS/ β -CD complex is more negative than those for 2AS/ α -CD, indicating a stronger and more stable interaction in β -CD. The negative Gibbs energy and enthalpy confirm spontaneous and exothermic complex formation, whereas negative entropy reflects reduced system disorder. The HOMO–LUMO energy gaps of the complexes suggest notable changes in the electronic structure and stability of 2AS upon molecular recognition and binding.

Table 2. Thermodynamic parameters for 2AS and its inclusion complexes by PM3 method.

Properties	2AS	α -CD	β -CD	2AS: α -CD	2AS: β -CD
E_{HOMO} (eV)	-8.13	-10.38	-10.35	-7.92	-7.99
E_{LUMO} (eV)	0.34	1.26	1.23	0.52	0.63
$E_{\text{HOMO}} - E_{\text{LUMO}}$ (eV)	-8.47	-11.63	-11.58	-8.44	-8.62
Dipole moment (D)	2.03	11.34	12.29	11.69	11.97
E (kJ/mol)	-65.06	-5219.62	-6098.72	-5407.86	-6001.36
ΔE (kJ/mol)				-121.04	-25.86
G (kJ/mol)	270.45	-2388.39	-2793.03	2604.21	3125.11
ΔG (kJ/mol)				-485.34	-602.50
H (kJ/mol)	385.35	-2829.93	-3303.35	3059.55	3528.87
ΔH (kJ/mol)				-614.96	-610.86
S (kJ/mol)	0.385	1.477	1.711	1.782	1.887
ΔS (kJ/mol)				-0.079	-0.210
ZPE*	69.96	635.09	740.56	703.46	808.36
Mullikan charge	0.00	0.00	0.00	0.00	0.00

ZPE = Zero point vibration energy

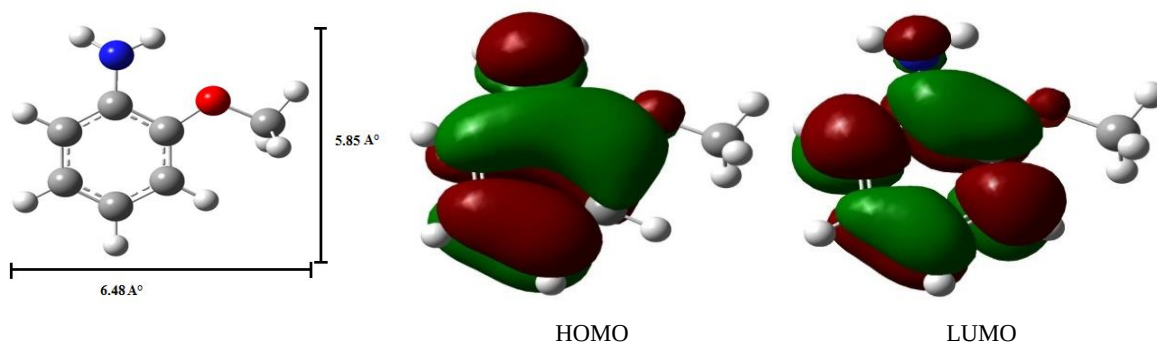


Figure 3. PM3 optimized structures of (a, b) 2AS (c, d) HOMO, LUMO of 2AS.

3.5. Nanomaterial Studies

3.5.1. Scanning Electron Microscope

The powdered samples of Cu nanoparticles, 2AS, and the Cu: 2AS: α -CD and Cu: 2AS: β -CD nanomaterials were examined using SEM (Figure 4). The Cu nanoparticles exhibit a clustered, ball-like morphology, while 2AS appears as

nanosheets. The Cu: 2AS: α -CD complex displays a nanocrystal-like structure, whereas the Cu: 2AS: β -CD complex shows a distinct nanorod morphology. SEM-EDX analysis confirms the elemental composition of the nanomaterials, revealing 55.6% carbon, 44.9% oxygen, and 0.98% Cu. The morphological variations among pure Cu nanoparticles, 2AS, and the inclusion complexes clearly support the successful formation of the Cu: 2AS: CD nanomaterials.

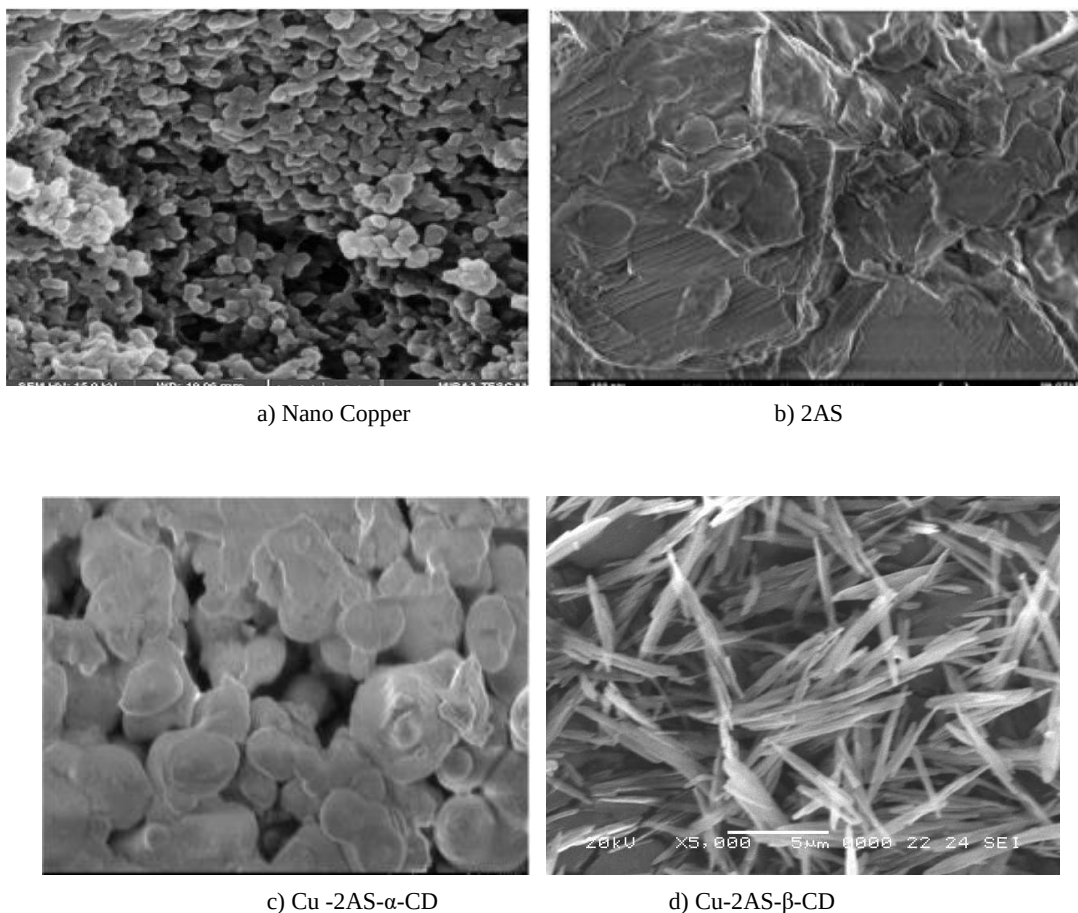


Figure 4. SEM images for a) Cu nano, b) 2AS, c) Cu: 2AS: α -CD and d) Cu: 2AS: β -CD.

3.5.2. Differential Scanning Colorimeter

The DSC thermograms of 2AS, α -CD, β -CD, Cu: 2AS: α -CD, and Cu: 2AS: β -CD inclusion complexes were analyzed. α -CD exhibits three endothermic transitions at 79.2, 109.1, and 137.5°C, while β -CD shows a broad endothermic peak at 128.6°C; these signals correspond to the loss of crystallization water from the CDs. Pure 2AS displays a sharp boiling point peak at 224°C and a melting endotherm at 6°C. In the inclusion complexes, α -CD, β -CD, and their respective Cu-containing systems show broader endothermic regions due to water loss. Notably, the Cu: 2AS: α -CD and Cu: 2AS: β -CD nanomaterials do not exhibit the characteristic peaks of free 2AS or CDs; instead, new thermal events appear at 252°C and

285°C, respectively, confirming the formation of new inclusion-based nanostructures.

3.5.3. Infrared Spectral Studies

FTIR analysis was performed for pure 2AS (Figure 5), α -CD, β -CD, Cu: 2AS: α -CD, and Cu: 2AS: β -CD nanomaterials. In free 2AS, the N–H stretching band appears at 3460 cm^{-1} , while N–H bending is observed at 1505 cm^{-1} . Aromatic C–H, C–O, and C=C stretching vibrations occur at 3060, 1303, and 1615 cm^{-1} , respectively. C–O–C and C–N stretching bands are located at 1225, 1130, and 1341 cm^{-1} . In the nanomaterials, NH_2 stretching shifts to 3271 cm^{-1} , and the aromatic C–H, C=C, and C–O stretching bands appear at 2905, 1415, and

1021 cm^{-1} , respectively. The disappearance of several characteristic peaks and the substantial reduction in band intensities

in Cu-2AS-CD complexes indicate successful doping of 2AS onto the copper nanoparticles.

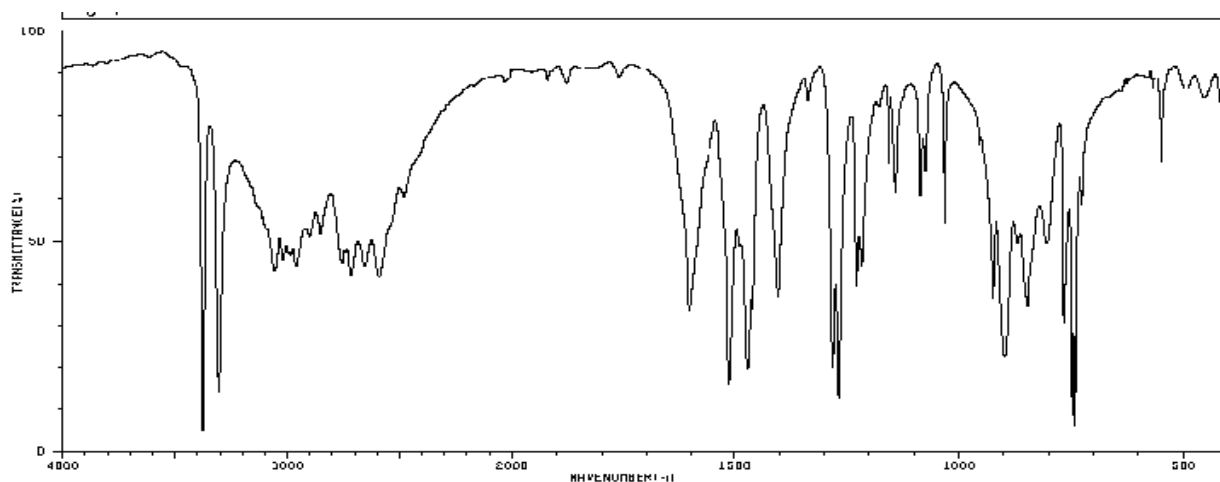


Figure 5. FTIR spectra of 2AS.

3.5.4. XRD Spectral Studies

The nanoparticles were assessed using XRD [41-50]. Pure Cu nanoparticles show diffraction peaks at 43.31° , 50.44° , and 74.20° , corresponding to reflections of the face-centered cubic (fcc) metallic structure. α -CD displays crystalline reflections at approximately 11.94° , 14.11° , and 21.77° , while β -CD exhibits peaks at 11.49° and 17.58° , though slight variation is possible depending on sample preparation. 2AS shows an amorphous pattern with a broad peak at 25.8° . The XRD pattern of Cu: 2AS: β -CD nanomaterials feature distinct diffraction peaks at 19.26° , 27.23° , 32.74° , 39.61° , 46.82° , and 74.78° . The changes in peak intensity and appearance relative to the pure components confirm the formation of new crystalline nanomaterial phases.

3.5.5. Proton Magnetic Resonance Spectral Studies

The ^1H NMR spectra of 2AS (Figure 6) and the nanomaterials were recorded in $\text{DMSO}-d_6$ at 25°C (Table 3). In CD-based inclusion complexes, the H-3 and H-5 protons—located inside the CD cavity—experience noticeable chemical shift variations due to interaction with the encapsulated 2AS molecule. Minor shifts are observed for H-1, H-2, and H-4 protons located on the outer rim of the CD. In general, guest molecules

incorporated into CD cavities show significant proton shift changes, consistent with the present results. For Cu: 2AS: CD nanomaterials, 2AS proton signals shift both upfield and downfield, accompanied by substantial reductions in peak intensity. These spectral features confirm strong interactions of 2AS with both the copper nanoparticles and the CD cavity protons, indicating successful formation of the Cu: 2AS: CD nanocomposites.

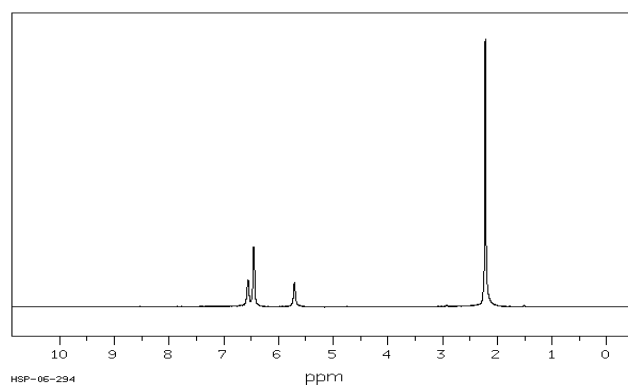


Figure 6. ^1H -NMR spectra of 2AS.

Table 3. ^1H -NMR chemical shift values for the 2AS and Cu: 2AS: α -CD nanomaterials.

Protons	2AS (δ)	Cu: 2AS: α -CD	Cu: 2AS: β -CD
H _a - para to OCH ₃	6.76	8.27	8.29
H _b -ortho to OCH ₃	6.74	5.69	5.71

Protons	2AS (δ)	Cu: 2AS: α -CD	Cu: 2AS: β -CD
H _c –Meta to OCH ₃	6.70	4.79	4.81
H _d –ortho to NH ₂	6.65	4.46	4.48
H _e -OCH ₃	3.77	2.48	2.50
H _f - NH ₂	3.70	2.05	2.07

4. Conclusion

At higher CD concentrations, the absorption and emission maxima of 2AS, as well as the overall spectral profiles in pH ~2, pH ~7, and pH ~11 solutions, differ markedly from those in water, indicating the formation of different types of inclusion complexes. While 2AS exhibits a single broad emission band in all solvents, dual emission is observed only at pH 11. The thermodynamic parameters of the 2AS: CD systems also deviate significantly from those of free 2AS, further confirming complex formation. SEM images clearly reveal distinct morphological differences between copper nanoparticles, 2AS, and the Cu-based nanocomposites. SEM–EDX analysis verifies the presence of copper within the nanomaterials. In the FTIR spectra of the Cu–2AS–CD complexes, several characteristic peaks disappear and pronounced reductions in band intensities are observed, supporting strong interactions between 2AS and the Cu–CD matrix. Additionally, in the 2AS: CD: Cu nanomaterials, the 2AS proton signals shift both upfield and downfield with substantial decreases in intensity, confirming the interaction of 2AS with both the copper nanoparticles and the CD cavity.

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
2AS	2-Anisidine
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: Supervision, Resources, Methodology, Software, Writing – original draft, Writing – review & editing

Ayyadurai Mani: Formal Analysis, Investigation

Palanichamy Ramasamy: Data curation

Sengamalai Senthilmurugan: Validation

Conflicts of Interest

The authors declare no conflict of interest.

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