

Synthesis Of Silver–3-Phenylenediamine–Cyclodextrin Nanomaterials And Ph-Dependent Characteristics Of 3-Phenylenediamine –Cyclodextrin Inclusion Complexes

N. Rajendiran, P. Ramasamy, P. Senthilraja, S. Senthilmurugan

Department Of Chemistry, Annamalai University, Annamalai Nagar, Tamilnadu, India

Molecular Biophysics Unit, Indian Institute Of Science, Bangalore, India

Department Of Bioinformatics, Bharathidasan University, Trichy - 620024, India

Department Of Zoology, Annamalai University, Annamalai Nagar, Tamilnadu, India

Abstract

The spectral characteristics of 3-phenylenediamine (3PDA) in various solvents, and in the presence of α -cyclodextrin (α -CD) and β -cyclodextrin (β -CD) at pH~3, and 7, were investigated using UV-visible, fluorescence, time-resolved fluorescence measurements, and PM3 computational methods. The 3PDA-CD-silver nanomaterials were synthesized and characterized by SEM, DSC, FTIR, XRD and ^1H NMR techniques. In all pH conditions, 3PDA exhibited distinct absorption and emission shifts upon complexation with α -CD and β -CD. In various solvents, the absorption and emission maxima of 3PDA were similar to those of 2-anisidine. 3PDA showed a single broad emission band in all solvents, whereas dual emission observed in CD solutions. The fluorescence lifetimes of the inclusion complexes were greater than that of free 3PDA. In the 3PDA molecule, both the vertical and horizontal bond lengths between the amino and hydroxy groups are smaller than the β -CD cavity size. SEM-EDX data confirmed the presence of 5.5% silver in the nanomaterials.

Keywords: 3-phenylenediamine, cyclodextrin, silver nano, pH effects, excimer.

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I. Introduction

The ability of cyclodextrins (CDs) to accommodate guest molecules of suitable size within their cavities has been widely utilized to control the photophysical and photochemical properties of various molecules, such as fluorescence enhancement and intramolecular excimer/exciplex formation [1–10]. Over the past two decades, we have investigated the solvent, pH, and CD dependences of the photophysical properties of various molecules [1–10] in both the ground and excited states. Since different organic molecules exhibit remarkable behavior depending on pH and microenvironmental conditions, it is worthwhile to study some substituted phenols under diverse conditions. In this context, we investigated the behavior of 3-phenylenediamine (3PDA) in the presence of α -CD and β -CD, which is used as model systems for studying cyclodextrin inclusion complexation. The present work focuses on: (i) To analyse absorption and fluorescence spectral shifts of 3PDA in α -CD, β -CD and solvents of different polarities (ii) proton-transfer behavior of 3PDA in aqueous, α -CD, and β -CD media; (iii) the structures and geometries of the inclusion complexes using PM3 molecular modeling; and (iv) the effect of doping of 3PDA:CD on Ag nanomaterial is analyzed through DSC, FTIR, ^1H NMR, and SEM techniques [1–10].

II. Materials And Methods

Preparation of CD Solution

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

Preparation of Ag:3PDA:CD Nanomaterials

A 0.01 M solution of silver nitrate was prepared in 50 mL of deionized water and warmed at 50–60 °C for 30 minutes. Then, 1–2 mL of 1% trisodium citrate solution (1 g dissolved in 100 mL of deionized water) was added with vigorous stirring. The appearance of a pale yellow color confirmed the formation of silver nanoparticles.

Cyclodextrin (1 mmol) was dissolved in 40 mL of distilled water, and 3PDA (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 using a magnetic stirrer. Subsequently, the silver nanoparticle solution was added and stirred for an additional 2 hours. The resulting dilute solution was gently warmed at 40–50 °C until its volume was reduced by approximately 50%. The solution was then refrigerated overnight at 5 °C.

The precipitated Ag-3PDA-CD nanomaterials were collected by filtration and washed several times with small amounts of ethanol and water to remove uncomplexed 3PDA, silver, and CD, respectively. The product was dried under vacuum at room temperature and stored in an airtight container. The resulting powder samples were used for further characterization and analysis [11-16].

III. Result And Discussion

Absorption and Fluorescence Spectral Results

Table 1 represent the absorption and emission spectral maxima of 3-phenylenediamine (3PDA) (2×10^{-4} M) in pH~3, and pH~7 solutions in different α -CD and β -CD concentrations. To compare the inclusion behavior of neutral and monocationic species of the 3PDA with CD, we studied the complexation behaviour of 3PDA at different pH solutions. In pH~7, the absorption and the emission maxima of the 3PDA resembles with the spectra observed in non-aqueous solvents and thus can be assigned to the molecular form of this molecule. The absorption and emission maxima of 3PDA in absence of CD with pH~3, and pH~7 aqueous solutions appear in the following wavelength: (pH~3: λ_{abs} ~276, 232 nm, λ_{flu} ~343 nm; pH~7: λ_{abs} ~288, 236 nm, λ_{flu} ~343 nm). The above results indicate that, the neutral species present in pH~7, whereas the blue shifted absorption maxima indicate monocation exists in pH~3. In both pH solutions, with increasing the α -CD concentrations, the absorption and emission maxima of the 3PDA decreased at the same wavelength, while blue shift (288 nm to 282 nm) noticed in the β -CD. In the higher α -CD and β -CD concentrations, the emission intensities completely quenched. In all the pH solutions, no significant emission shift observed in the α -CD/pH~3 and α -CD/pH~7 solution, while blue shift (345 nm to 340 nm) noticed in the β -CD. In the absence and presence of α -CD and β -CD solutions, the absorption and emission maxima and spectral shape of 3PDA in pH~3 is different from pH~7 buffer solutions.

Different change observed in the absorption and emission intensities and the spectral maxima are owing to the encapsulation of 3PDA molecule into the α -CD and β -CD cavities [16-30]. Further, no noteworthy changes were observed in the absorbance of these solutions when recorded after 12 hrs. The binding constant (K) values were obtained from the slope and the intercept of the Benesi-Hildebrand equation (Table 1). This analysis reflects the formation of 1:1 inclusion complex between 3PDA:CD. As can be seen from the Table 1, ΔG is negative which suggests that the inclusion proceeded simultaneously at 303K and it is an exothermic process. The binding constants are very sensitive to change of pH support the selective inclusion associated with the 3PDA (neutral and monocation) species.

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

Concentration of CD $\times 10^{-3}$ M	pH - 3				pH - 7			
	λ_{abs}	log ϵ	λ_{flu}	τ	λ_{abs}	log ϵ	λ_{flu}	τ
3PDA only (without CD)	276 232	3.54	345	0.025	288 236	3.58	345	0.025
0.2 α -CD	276 232	3.50	344	0.032	288 236	3.54	344	0.035
1.0 α -CD	276 232	3.29	344	0.41	288 236	3.32	344	0.45
0.2 β -CD	277 231	3.46	344	0.036	284 232	3.52	340	0.041
1.0 β -CD	277 231	3.37	340	0.48	282 232	3.46	340	0.52
Excitation wavelength (nm)			270				270	
K (1:1) $\times 10^5$ M ⁻¹ α -CD	101		378		588		813	
ΔG (kcal mol ⁻¹) α -CD	-11.63		-14.95		-16.07		-16.88	
K (1:1) $\times 10^5$ M ⁻¹ β -CD	444		686		396		672	
ΔG (kcal mol ⁻¹) β -CD	-15.37		-16.46		-15.07		-16.40	

To check the entrapment of the 3PDA into the CD, we also studied the solvent provoked changes in the absorption and emission spectra for this molecule in selected solvents (cyclohexane: λ_{abs} ~293, 240 nm, λ_{flu} ~320 nm; acetonitrile: λ_{abs} ~297, 240 nm, λ_{flu} ~326; methanol: λ_{abs} ~292, 238 nm, λ_{flu} ~ 335; water: λ_{abs} ~288, 235 nm, λ_{flu} ~340 nm). In all the solvents, α -CD and β -CD, 3PDA gives single emission maximum only and the absence of longer wavelength emission in 3PDA indicates that ICT or exciplex or excimer is not formed in all the solvents.

Compared to aniline (cyclohexane: λ_{abs} ~283, 235 nm, λ_{flu} ~320 nm; acetonitrile: λ_{abs} ~286, 238 nm, λ_{flu} ~329; methanol: λ_{abs} ~284, 232 nm, λ_{flu} ~ 334; water: λ_{abs} ~278, 230 nm, λ_{flu} ~335 nm) the absorption and emission maxima of 3PDA are red shifted in all the solvents suggest, both amino groups interact with the phenyl ring.

Excited Singlet State Lifetimes

To examine the CD provoked changes in the fluorescence spectra of 3PDA, the emission decay of the emissions in aqueous α -CD and β -CD solutions were analysed (Table 1). In 3PDA, biexponential decay was noticed in water, α -CD and β -CD. The decay behavior of 3PDA indicates the existence of the single emitting species in 3PDA molecule. The lifetimes of the guest: host inclusion complexes were higher than that of the isolated guest molecules. The increase in the lifetime value with increase in CD concentration is due to the encapsulation of the 3PDA in the CD cavity. The life time of the 3PDA increased in the following order: water < α -CD < β -CD. This order indicates that β -CD:3PDA inclusion complex has more stable than α -CD inclusion complexes. This reflects that the 3PDA: α -CD inclusion complex is quite different from that of the 3PDA: β -CD complexes.

Molecular Modeling

The ground state geometries of 3PDA and CDs were optimized using PM3 method (Fig. 1). HOMO, LUMO, thermodynamic parameters (energy, enthalpy, entropy and free energy), dipole moment, zero point vibrational energy and Mulliken charge of the 3PDA, α -CD and β -CD and inclusion complexes are summarized in Table 2.

Both CDs heights are same (7.8 Å), the interior cavity size of α -CD is 4.7- 5.3 Å and β -CD is 6.0 - 6.5 Å and the exterior cavity size of α -CD is 8.8 Å and β -CD is 10.8 Å. In 3PDA, the vertical and horizontal bond distance between NH₂ – aromatic ring is 5.85 Å and 5.43 Å respectively (Fig. 1). In 3PDA, both vertical and horizontal bond length between the amino and aromatic ring hydrogen is lower than α -CD and β -CD cavity size, hence the guest molecule may fully be entrapped into the inside of the CD cavity. The above results indicate that, 3PDA can form different types of inclusion complexes in the α -CD and β -CD. Further, the optimized structures of the inclusion complexes were also confirmed that the 3PDA molecule partially included in the CD cavity. The results show that in CD, the geometry of the 3PDA is slightly altered. The optimized theoretical structure of the CD:3PDA inclusion complexes also confirmed that the 3PDA molecule is included in the CD cavity.

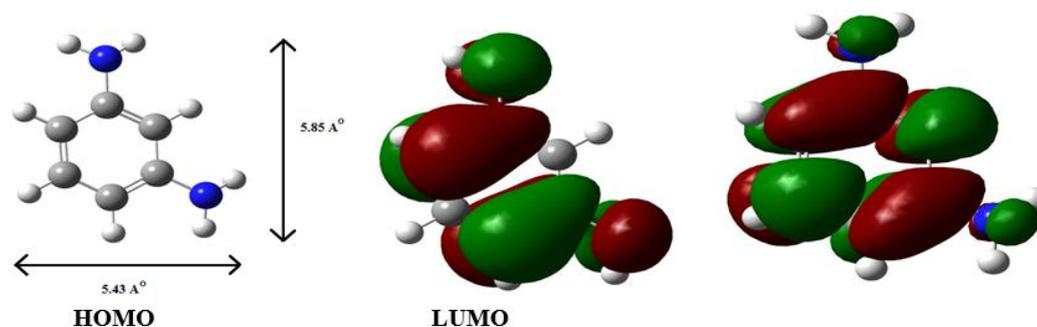


Fig. 1 PM3 optimized structures of (a, b) 3PDA (c, d) HOMO, LUMO of 3PDA

The thermodynamic parameter ΔG for the formation of the guest molecule to both CDs are negative which suggests that the inclusion proceeded simultaneously and the inclusion reactions were exothermic process at 303 K. HOMO, LUMO, energy, free energy, enthalpy, entropy, dipole moment and zero point vibration energy of the CD:3PDA is appreciably changed than the isolated 3PDA molecule indicates inclusion complex is formed. The polarity of the CD changed after the 3PDA entered in to the CD cavity. The negative energy, enthalpy and Gibbs free energy changes suggested that the inclusion processes were energetically and enthalpically favourable in nature. The binding energy (ΔE) of the inclusion complexes are higher than that of isolated 3PDA molecule suggesting that stability of complexes is more. The negative ΔH values indicated that the inclusion formation of 3PDA with CD is an exothermic and enthalpy driven. The small negative ΔS value is due to enhancement of disorder in the system. Moreover, hydrophobic interactions, which are long range interactions, can be important in the CD complex formation. Comparison of ΔH and ΔS confirm that enthalpy change is higher and entropy changes are lower for the complexation. Therefore, the inclusion complex of 3PDA with CD is more enthalpy stabilized.

Table 2. Binding energies and HOMO, LUMO energy of 3PDA with α -CD and β -CD by PM6 method.

Properties	3PDA	α -CD	β -CD	3PDA- α -CD A	3PDA- α -CD B	3PDA- β -CD A	3PDA- β -CD B
E_{HOMO} (eV)	-8.20	-10.05	-9.99	-8.62	-8.21	-8.11	-8.64
E_{LUMO} (eV)	0.67	0.14	0.12	0.17	0.24	0.24	0.21
$E_{\text{HOMO}} - E_{\text{LUMO}}$ (eV)	-8.88	-10.19	-10.11	-8.79	-8.46	-8.35	-8.85
μ (eV)	-3.76	-4.95	-4.93	-4.22	-3.98	-3.93	-4.21
χ (eV)	3.76	4.95	4.93	4.22	3.98	3.93	4.21

η (eV)	4.25	5.09	5.05	4.39	4.22	4.17	4.42
S (eV)	2.12	2.54	2.52	2.19	2.11	2.08	2.21
ω (eV)	3.59	4.81	4.81	3.83	3.73	3.67	3.72
Dipole (D)	2.63	9.92	10.52	3.65	4.09	10.03	8.59
E^*	16.98	-1353.95	-1577.74	-1350.21	-1351.11	-1572.19	-1570.56
ΔE^*				-13.24	-14.13	-11.43	-9.80
G^*	58.26	510.13	606.37	586.39	584.62	680.32	679.58
ΔG^*				17.99	16.22	15.69	14.95
H^*	83.12	599.76	704.03	680.96	681.34	785.28	785.19
ΔH^*				-1.92	-1.54	-1.87	-1.97
S^{**}	83.40	300.59	327.58	317.19	324.40	352.04	354.21
E^*				-66.80	-59.59	-58.94	-56.77

* kcal mol⁻¹ ** kcal/mol-Kelvin

Inclusion Complex Nanomaterial Studies

Field Emission Scanning Electron Microscopy

The powdered form of Ag nano, 3PDA and Ag:3PDA: α -CD and Ag:3PDA: β -CD nanomaterials were investigated by FE-SEM (Fig. 2). These pictures clearly show, Ag nano present in ball shape, 3PDA in sheet shape, Ag:3PDA: α -CD and Ag:3PDA: β -CD are in stick shape. SEM EDEX data confirm 39.86% carbon, and 60.10 % Ag present in the nanomaterials. The different structure of the Ag nano, and 3PDA supports the formation of the Ag-3PDA-CD nanomaterials.

Differential Scanning Colorimeter

The DSC curves of α -CD show three endothermic peaks at 79.2 °C, 109.1 °C and 137.5 °C and β -CD shows a broad endothermic peak at 128.6 °C and, these endothermic peaks are attributed to loss of water from CDs. The boiling point of 3PDA shows a sharp peak at 284 °C and the melting point is 64 °C. A broader endothermic effect was recorded for α -CD, β -CD and the respective nanomaterials as a consequence of water loss from the CDs. The DSC thermogram of the nanomaterials did not show peaks corresponding to pure 3PDA and CD, instead new peaks appeared at 255 °C and 276 °C for 3PDA: α -CD and 3PDA: β -CD respectively.

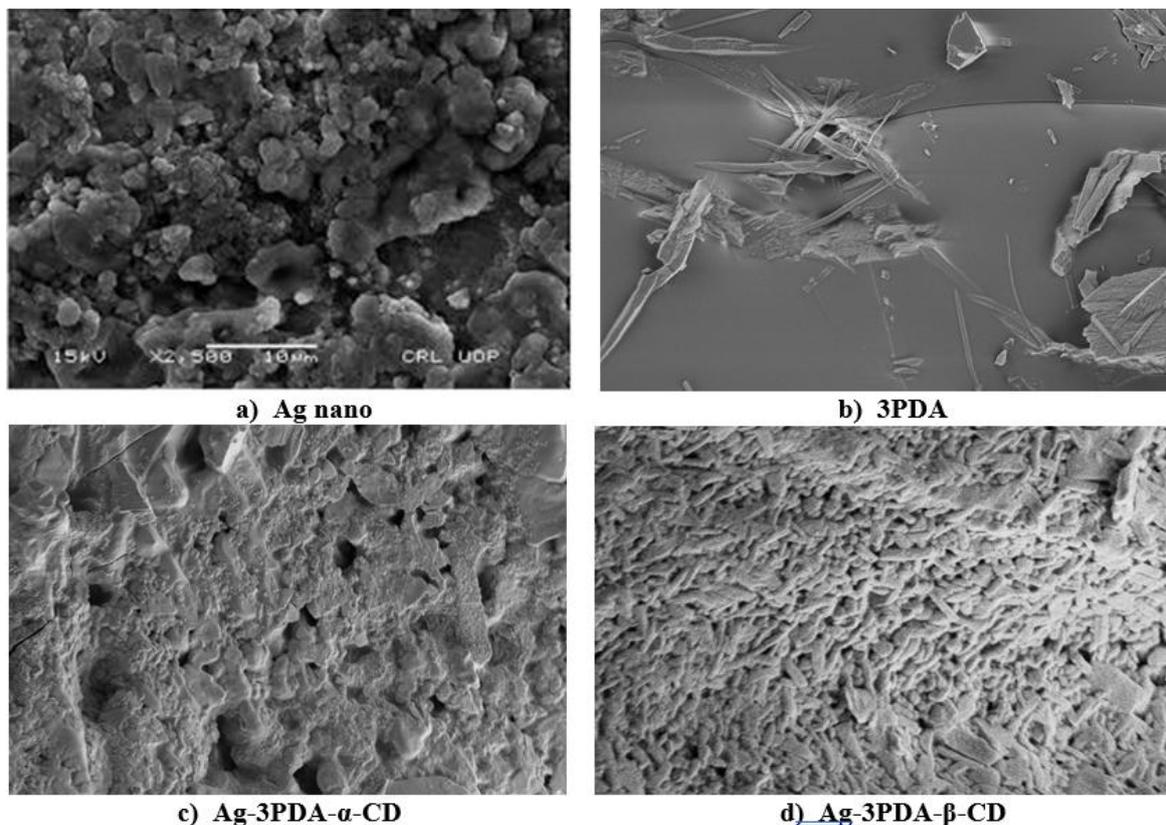


Fig. 2 SEM images of (a) 3PDA, (b) Ag:3PDA: α -CD nano, (c) Ag:3PDA: β -CD nano.

Infrared Spectral Studies

FTIR spectra of the Ag:3PDA:CD nanomaterials compared to pure Ag nano, α -CD, β -CD and 3PDA. In 3PDA, the NH₂ stretching frequency appears at 3322 cm⁻¹. The aromatic C=C, and C-C stretching frequency appears at 992 cm⁻¹ and 953 cm⁻¹ respectively. The aromatic C-N stretching frequency appears at 1310 cm⁻¹. In the Ag:3PDA:CD nanomaterials, the NH₂ stretching frequency appears at 3325 cm⁻¹ and the aromatic C=C and C-C stretching frequency appears at 940 cm⁻¹ and 842 cm⁻¹ respectively. The aromatic C-N stretching frequency appears at 1387 cm⁻¹. In Ag:3PDA:CD, the Ag stretching frequency appears at 753 cm⁻¹ respectively. Most of the frequency was not appeared and significant decrease in intensity was noted suggest that the 3PDA molecule interact with silver nano and CD.

¹H NMR Spectral Studies

In order to comprehensively examine the structures of 3PDA and the CD complexes were investigated by ¹H-NMR. ¹H-NMR spectra of 3PDA and the inclusion complexes are performed at 25 °C in DMSO-*d*₆. Both amino protons appear at 3.53, both 4th and 6th position ortho protons appear at 6.075 (doublet), the meta 5th position proton appear at 6.912 (singlet) and the 2nd position proton appear at 5.95. Generally, the chemical shift values of the 3PDA protons tend to show appreciable changes if the guest molecules are included in the CDs cavities. The chemical shift value of 3PDA protons are shifts to up field in the both CD complexes. These results indicate that all the protons of 3PDA are interacting with CD cavity protons.

X-RD Spectral Studies

XRD analysis confirmed the formation of nanomaterials. Based on JCPDS data, the mineral name (3C) and face-centered cubic (FCC) structure were identified. The standard FCC structure corresponds to JCPDS card number 87-0717, with hkl values at 111, 200, 220, and 311. Ag nanoparticles showed four distinct peaks at $2\theta = 38.11^\circ, 44.30^\circ, 64.45^\circ, \text{ and } 77.40^\circ$. 3PDA showed the following peaks at $2\theta^\circ = 12.4, 19.2, 27.3, 38.0, 44.4, 46.0 \text{ and } 77.84^\circ$, while several peaks were observed for Ag/3PDA/ β -CD at $2\theta^\circ = 15.2, 18.8, 20.2, 21.3, 22.1, 23.6, 26.1, 27.0, 29.4, 35.1, 44.4, 46.2, \text{ and } 77.8^\circ$. The XRD patterns of Ag/3PDA/ β -CD exhibited distinct diffraction features, confirming the formation of new nanomaterials. The appearance of additional peaks and variations in intensities further support the formation of novel nanomaterials.

IV. Conclusion

Absorption and emission spectral maxima of 3-phenylenediamine (3PDA) in different α -CD and β -CD concentrations with *pH*~3 and *pH*~7 solutions were investigated. In all the solvents, α -CD and β -CD solutions, the absorption and emission maxima and spectral shape of 3PDA in *pH*~3 is different from *pH*~7 buffer solutions. 3PDA gave a single broad emission spectrum in all the solvents. 3PDA gives single emission maximum in α -CD but dual emission in β -CD. The different spectral change of 3PDA with addition of CD in the *pH*s suggest that the structural geometry of the inclusion complexes are different in terms of orientation of guest molecule. The increase in the lifetime value with increase in CD concentration is due to the encapsulation of the 3PDA in the CD cavity. This lifetime values indicates that β -CD:3PDA inclusion complex has more stable than α -CD inclusion complexes. SEM pictures and EDEX data confirm 34.2% carbon, 44.2% oxygen and 21.6% nano Ag present in the nanomaterials. DSC thermogram of Ag:3PDA:CD complexes did not show peaks corresponding to pure 3PDA and CD, instead new peaks appeared for the nanomaterials. The chemical shift value of 3PDA protons are shifts to up field and down field and the peak intensities are very low in the nano Ag with CD nanomaterials. These results indicate that all the protons of 3PDA are interacting with Ag nano and CD cavity protons.

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