

## Investigations of CTAB Assisted Cadmium Complex: An Organometallic Compound for Organic Light Emitting Diode Applications

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A novel route was employed for the synthesis of pure and guest surfactant (CTAB) assisted cadmium[(2-(2-hydroxyphenyl)benzoxazole)-(8-hydroxyquinoline)] having composition Cd(HPB)q nanorods, where HPB = 2-(2-hydroxyphenylbenzoxazole) and q = 8-hydroxyquinoline. Powder X-ray diffraction analysis was used for structural analysis and to calculate the particle size using Scherrer equation. Fourier transform infrared spectroscopy was employed to confirm the composition of Cd(HPB)q. Scanning electron microscope images indicated that lower temperature and a shorter reaction time would be suitable for the formation of nanorods. UV-vis-NIR spectroscopy was used to determine the band gap energies of Cd(HPB)q complexes. Photoluminescence spectra showed a prominent peak around 500 nm, which indicated a strong photoluminescence emission in the green region making the complex a promising organic light emitting diode (OLED) candidate.

**Keywords:** Organic Light Emitting Diode, Surfactant, CTAB.

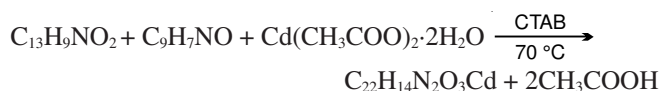
### INTRODUCTION

In organic light emitting diodes (OLEDs), green light emitters have attracted much attention due to their stability and brightness [1,2]. The need for stable and efficient light emitting molecules becomes obvious due to the growing market of organic light-emitting diodes. Organic light emitting diodes (OLEDs) with low molecular weight electroluminescent materials are promising candidates for lighting applications due to their low power consumption, wide viewing angle and ease of fabrication [3,4]. These small molecules had been synthesized by many groups by taking different metals like aluminum, zinc, iridium, gadolinium, europium, platinum, *etc.* along with different ligands, like 2-(2-hydroxyphenylbenzoxazole), 8-hydroxyquinoline, 1,10-phenanthroline, 2,2'-bipyridine, *etc.* [5-7]. Nowadays cadmium complexes have been synthesized by different groups for their use in OLED applications due to their thermal stability, simplicity in synthesis procedure and wide spectral range. Extensive research work is going on to synthesize new cadmium complexes containing new ligands to produce a number of novel luminescent cadmium complexes as emitters and electron transporters in OLED applications [8-10]. The coordination numbers of cadmium complexes are variable, making it possible to synthesize new emitter materials with varying

optoelectronic properties [11-13]. In this paper, we report the synthesis of cadmium[(2-(2-hydroxyphenyl)benzoxazole)-(8-hydroxyquinoline)], Cd(HPB)q by a simple novel method and the effect of surfactant CTAB (0.5%) on its structural, morphological, optical and photoluminescence properties.

### EXPERIMENTAL

**Synthesis:** A solution of 2-(2-hydroxyphenyl)benzoxazole (HPB) with 0.211 g (1 mmol) (Merck, India) was prepared in 20 mL of absolute ethanol in a 100 mL three neck flask and stirred with 0.5 % of CTAB using a magnetic stirrer for 1 h at 70 °C. Then the solution of cadmium acetate dihydrate 0.267 g (1 mmol) in 3 mL of water and 8-hydroxyquinoline (q) 0.145 g (1 mmol) in 10 mL absolute ethanol was added dropwise in the above solution under constant stirring. After the complete addition of alcohol, the reaction was further carried out for 3 h. The yellow precipitate formed was filtered and dried overnight [14].



Reaction Scheme for the synthesis of [Cd(HPB)q]

## RESULTS AND DISCUSSION

**Powder X-ray diffraction analysis:** The powder X-ray diffraction patterns for the synthesized samples are shown in Fig. 1. The sharp distinct peaks indicate the crystalline nature of cadmium complex. The strong diffraction peaks in the XRD spectrum occurring at  $2\theta$  values of the complex at 11.96, 16.35, 20.75, matches with the peaks of 8-hydroxyquinoline, 24.33, 26.93, 28.91 of 2-(2-hydroxyphenyl)benzoxazole (HPB) and 34.71 and 47.71 for cadmium acetate [15]. Fig. 2 represents the introduction of CTAB. It clearly indicates that the sharp peaks in pure material have been absent and this explains that surfactant employed have been masking the other peaks in the cadmium complex. The prominent peaks observed from the X-ray diffraction patterns were used to calculate the particle size *via* the Scherrer equation. The particle sizes were found out to be 68 and 64 nm for pure and CTAB assisted Cd[HPB]q, respectively.

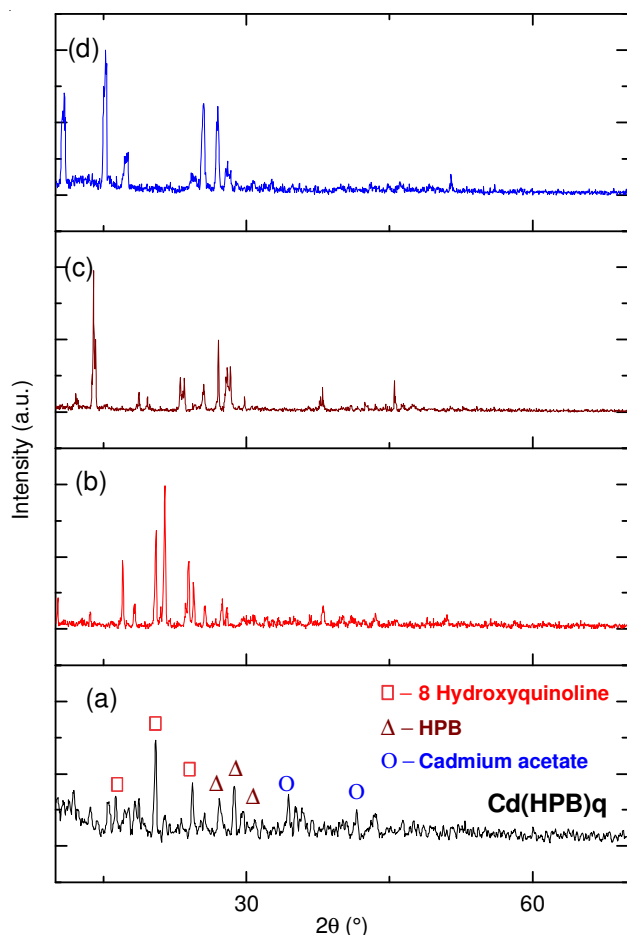


Fig. 1. X-ray diffractogram for (a) Cd(HPB)q complex (b) 8-hydroxyquinoline (c) HPB and (d) cadmium acetate

**SEM analysis:** Fig. 3(a, b) shows the SEM micrographs of as-synthesized pure, CTAB assisted cadmium complexes. The pure cadmium complex is composed of branched aggregates of nanorods. A close observation of SEM image of the present case suggests that the surfaces of the nanorods are relatively smooth and this could be attributed to the relatively low reaction temperature employed. It revealed that CTAB played an important role in preventing the agglomeration of the cadmium

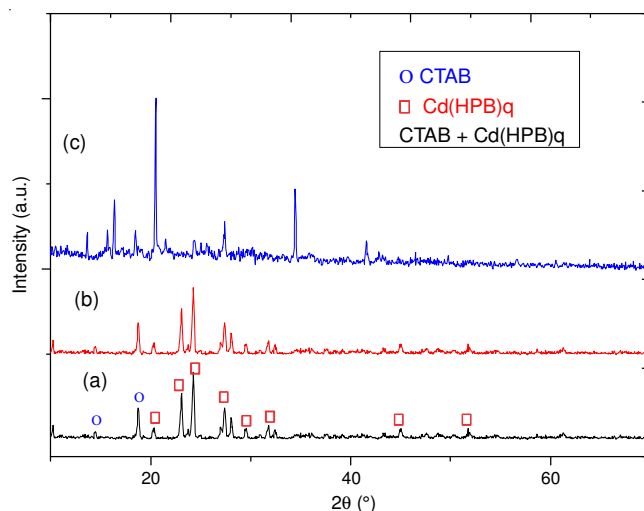


Fig. 2. X-ray diffractogram for (a) CTAB+Cd(HPB)q complex (b) Cd(HPB)q complex and (c) CTAB

complex. In the formation process of the shape evolution of cadmium complex, the surfactant CTAB is absorbed onto the different planes of cadmium complex and it not only prevents the particles from agglomeration, but shows more homogenous surfaces.

**EDAX analysis:** EDAX is an important technique to analyze the composition of elements quantitatively and solve the chemical identity of any nanomaterial. It is inferred from the result of the EDAX spectra that the samples are composed of only cadmium and no trace of other elements is observed. Though, two different organic species were employed, the peaks related to organic surface is not visible and it is clear that the samples are generally cadmium rich. Fig. 3(c and d) shows the signs of carbon at 0.2ev, oxygen at 0.6ev and cadmium at 3.2ev, respectively.

**FTIR analysis:** Fig. 4 shows the FTIR spectra of cadmium complex synthesized in the absence and presence of the surfactant CTAB dispersed in KBr powder. The FTIR spectra were recorded in the range 4000–400  $\text{cm}^{-1}$ . Table-1 shows the FTIR assignments made for the complex. Similarity observed in the FTIR spectra of both indicated that there is similar composition and structure for the cadmium complex prepared in the absence and presence of surfactant CTAB. However, the characteristic peak of CTAB is not observed in the spectrum. In case of Cd(HPB)q, the absorptions at 1600, 1570, 1495  $\text{cm}^{-1}$  corresponds to C=C stretching of phenyl ring. The bands at 1321 and 1279  $\text{cm}^{-1}$  corresponds to C=N stretching. The band at 1106  $\text{cm}^{-1}$  is assigned to C-O bond stretching. The band at 760 and 735  $\text{cm}^{-1}$  represent the C-H wagging of aromatic rings with 3 and 4 adjacent hydrogen atoms respectively in the aromatic ring. The bands at 576 and 493  $\text{cm}^{-1}$  correspond to cadmium oxygen stretching and 462  $\text{cm}^{-1}$  correspond to cadmium-nitrogen stretching, respectively [16].

TABLE-1  
FTIR ASSIGNMENTS OF Cd(HPB)q

Assignments	Wavenumber ( $\text{cm}^{-1}$ )
Aromatic C=C Stretching	1600, 1570, 1495
C=N stretching	1321, 1279
C-O stretching	1106
Aromatic C-H wagging	760-735
Cd-O bond stretching	576
Cd-N bond stretching	493, 462

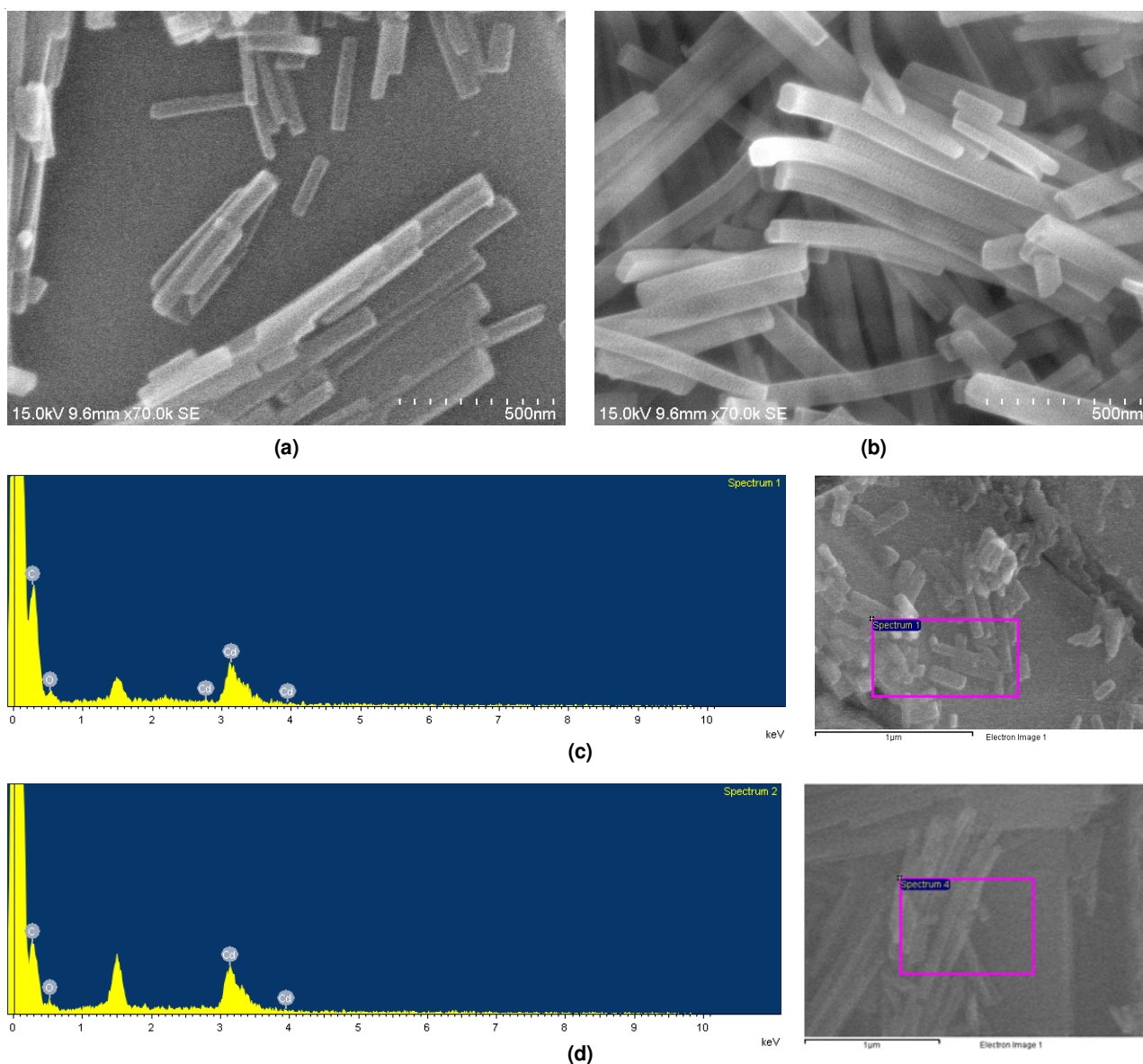


Fig. 3. SEM [(a) pure, (b) CTAB] and EDAX [(c) pure, (d) CTAB] analysis of cadmium complexes  $[\text{Cd}(\text{HPB})\text{q}]$

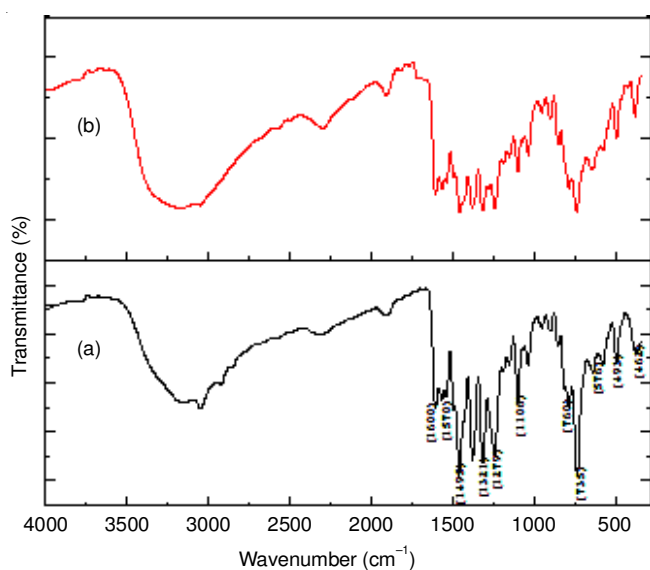


Fig. 4. FTIR spectra of (a) pure, (b) CTAB assisted cadmium complexes  $[\text{Cd}(\text{HPB})\text{q}]$

**UV-vis-NIR analysis:** The controlling and tuning of band

edge emission and surface traps state emission of cadmium complex are obviously very important to realize the tunable optical properties. The UV-vis-NIR spectral analysis was carried out between 200 nm and 800 nm. Fig. 5 shows the absorption spectra of cadmium complex pure and surfactant assisted nanoparticles. The relatively sharp absorption indicates the narrow size distribution of the nanoparticles. In the case of CTAB assisted cadmium complex, the absorption band edge is shifted to 470 nm and the corresponding band gap is 2.61 eV. Thus, it is clear from the optical absorption study that the assisted cadmium complex with organic surfactant of CTAB modifies the band gap of the complex and the sample is blue shifted in the spectrum when compared to the pure complex.

**Photoluminescence analysis:** The photoluminescence studies on cadmium complex have been investigated and are shown in Fig. 6.  $\text{Cd}(\text{HPB})\text{q}$  with CTAB showed similar photoluminescence characteristics. The yellow coloured complex with cationic surfactant exhibited a single emission band ranging from 500–520 nm, respectively. It has been observed that the

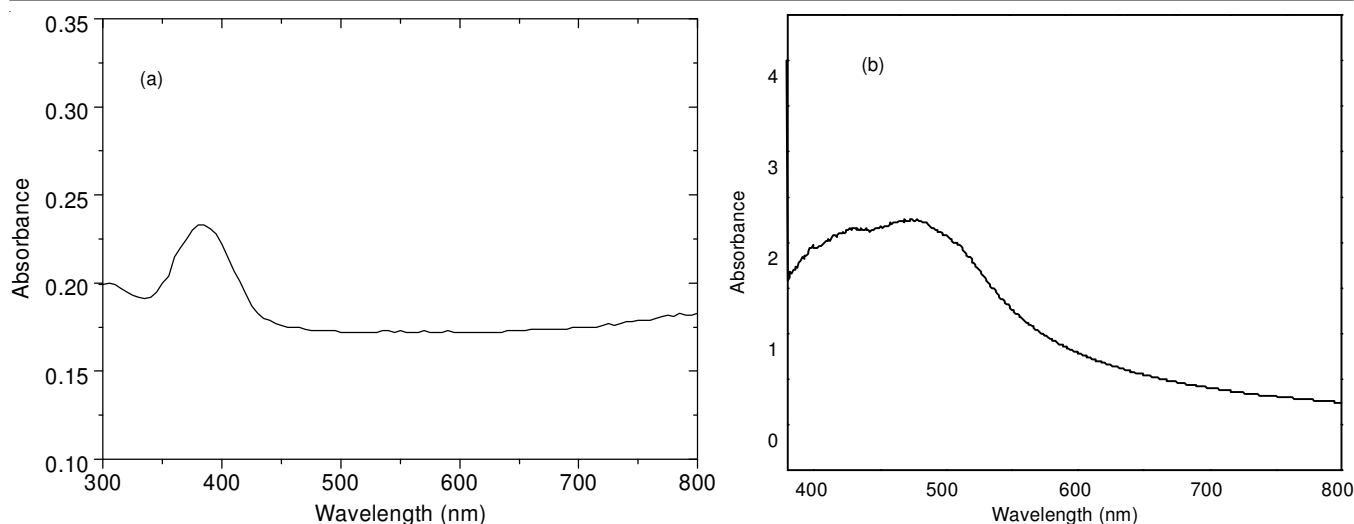


Fig. 5. Absorption spectra for (a) pure, (b) CTAB assisted cadmium complexes [Cd(HPB)q]

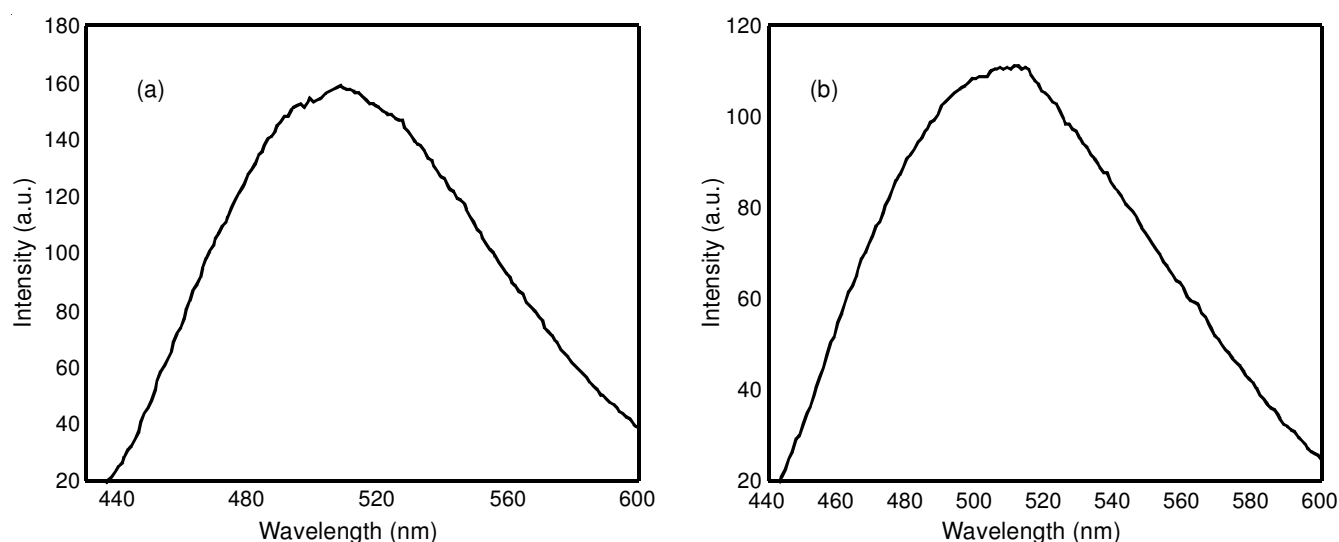


Fig. 6. Photoluminescence spectra of (a) pure, (b) CTAB assisted cadmium complexes [Cd(HPB)q]

presence of a emission peak at 508 nm and 518 nm for pure and CTAB assisted indicated a strong emission in the green region.

## Conclusion

A novel method has been followed in synthesizing pure and CTAB assisted cadmium complex by the reaction of 8-hydroxyquinoline and 2-(2-hydroxyphenyl)benzoxazole with cadmium acetate. The peaks corresponding to  $2\theta$ s 24.7, 28.3, 36.4 and 43.6 ascertain the phase of cadmium complex. A close observation of SEM image of the present case suggests that the surfaces of nanorods are relatively smooth and this could be attributed to the relatively shorter reaction time and lower temperature employed. Though, two different organic species were employed, the peaks related to organic surface is not visible and it is clear that the samples are generally cadmium rich. The FTIR spectra of both indicated that there is similar composition and structure for the cadmium complex prepared in the absence and presence of surfactant CTAB. In case of Cd(HPB)q the absorptions at 1600, 1570, 1495  $\text{cm}^{-1}$  corresponds to C=C stretching of phenyl ring. The bands at 1321, 1279

$\text{cm}^{-1}$  corresponds to C-N stretching. The band at 1106  $\text{cm}^{-1}$  is assigned to C-O bond stretching. The band at 760 and 735  $\text{cm}^{-1}$  represent the C-H wagging of aromatic rings with 3 and 4 adjacent hydrogen atoms, respectively in the aromatic ring. The bands at 576 and 493  $\text{cm}^{-1}$  correspond to cadmium oxygen stretching and 462  $\text{cm}^{-1}$  correspond to cadmium nitrogen stretching, respectively. The relatively sharp absorption indicates the narrow size distribution of the nanoparticles. In the case of CTAB assisted cadmium complex the absorption band edges are shifted to 380 nm and the corresponding band gap is 2.61 eV, respectively. The photoluminescent spectra showed a prominent peak around 500 nm which indicated a strong photoluminescent emission in the green region.

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