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FTIR Spectoscopy of Ca⁺⁺ DOPED Alq₃ OLED Phospor

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Abstract: Pure Ca^{++} alkaline earth metal element doped Alq_3 Complex was synthesized by simple precipitation method at room temperature, maintaining stochiometric ratio. Complex was characterized by XRD and FT-IR spectra. XRD analysis reveals the polycrystalline nature of the synthesized complex. FT-IR is an analytical technique which confirms the molecular structures of the synthesized complexes. FT-IR results confirm the completion of quinoline ring formation and presence of quinoline structure in the metal complex. Thus, prepared phosphors can be a suitable candidate in ultraviolet visible region for emitting OLED, PLLCD, solid state lighting applications and ultrasonic applications.

Keywords: Alkaline earth metal elements, metal complexes, FTIR spectroscopy, OLED.

1. Introduction

Organic light emitting materials have been attracting attention of researchers from industry and academic institutions owing to their applications in OLEDs [1], stimulating interest in next-generation displays and lighting technologies [2]. The efficient and stable tri (8hydroxyquinoline) aluminum (Alq₃) is extensively investigated because of its high stability, good emission, easy synthesis, electron transport properties and high quantum efficiency. Alq₃ is used as electron transporting layer, as emission layer where green light emission is generated by electron hole recombination in Alq₃. It is also served as host material for various dyes to tune emission color from red to green [3]. Although Alq3 has low fluorescence efficiency, it has excellent properties as emitting material, namely high stable film forming, high carrier transport and good heat resistance. Tang and coworkers fabricated Alq_3 based multi-layer thin film electro-luminescent devices in 1987 [4, 5and 6]. Alq₃ still continues to be the workhorse among the class of low molecular weight materials for OLED.

Alkaline earth element Ca⁺⁺ doped play vital role in the enhancement of PL intensity with small change in PL emission wavelength. Hence it is proposed to synthesize and characterize strontium doped Alq₃, which is generally used as electron transport or emission layer strontium doped Alq₃ [7]. The investigation of Ca^{++} doped Alq₃ is carried out by using FTIR spectroscopy.

2. Experimental

Synthesis of Ca⁺⁺ doped Alq₃

Tris (8-hydroxyquinolinato) aluminum is the chemical compound with the formula $Al(C_9H_6NO)_3$, widely abbreviated Alq₃. 5 gm. of HQ (8-hydroxy quinoline) was dissolved in 25 ml of distilled water and 25 ml acetic acid. The solution was heated to 50°C for 30 min and filtered to remove insoluble impurities. For pure Alq₃, 4.3069 gm of 3Al(NO₃)₃ 9H₂O was dissolved in 100 ml of distilled water. This solution was also heated to 50 ^oC for 30 min. Later the hydroxyl quinoline solution was slowly added to the above solution. Yellow precipitate was obtained. To this NH₄OH₄ was added to get the maximum yield. The yellow precipitate was then filtered and washed with warm water until the filtered water became colorless. Finally, it was dried at 60° C for 2 hr in order to remove water molecules. The other derivative of 8-hydroxyquinoline metal complexes Alq₃ were synthesized by the same procedure, just by replacing aluminum nitrate by Calcium acetate mixed in an appropriate molar ratio.

Chemical reactions of synthesis process are as follows

$$A1(NO_3)_3.9H_2O + 3 (C_9H_7NO) \longrightarrow A1(C_9H_7NO)_3 + 9H_2O + 3(NO_2)$$

Al(NO₃)₃.9H₂O + (CH₃COO)₂Ca.4H₂O+3 (C₉H₇NO) -----

 $A1Ca(C_9H_7NO)_3 + 2(CH_3COOH) + 12H_2O + 2O_2 \uparrow + 3(NO_2) \uparrow$

In the synthesis process, when calcium metal is added, it contributes an electron, withdrawing constituent at the 5position in 8-hydroxyquinoline, thereby increasing the solubility of the corresponding metal quinolate complexes in non-polar solvents.

3. Results and Discussion

The synthesized complex has been characterized by XRD on The 'Expert pro' Automated power Diffractometer system company name "Analytical", Netherland and FTIR spectroscopy was taken on IR spectrum of Ca⁺⁺ doped Alq₃ samples was measured on KBr pellets in a Perkin Elmer LR 64912C Fourier transform infrared (FT-IR) spectrometer with KBr beam splitters and a resolution of 20cm⁻¹ at 'SAIF' Punjab University, Chandigarh.

3.1. X-ray Diffraction

X- Ray Diffractogram of Ca^{++} doped Alq₃ exhibits well defined X-ray diffraction lines for the powder sample that confirm its crystalline nature. The presence of distinct lines confirmed the polycrystalline nature of the synthesized complex as shown in Fig. 1.



Figure 1: X-ray Diffractogram of Ca⁺⁺ doped Alq₃

3.2. FTIR spectroscopy of Ca⁺⁺ doped Alq₃

FT-IR is an analytical technique which confirms the molecular structures of the synthesized complexes. This technique measures the absorption of various infrared light wavelengths by the material of interest. In order to probe the structural transformation of Ca⁺⁺ doped Alq₃, IR spectrum of Ca⁺⁺ doped Alq₃ samples was measured on KBr pellets in a Perkin Elmer LR 64912C Fourier transform infrared (FT-IR) spectrometer with KBr beam splitters and a resolution of 20cm^{-1} . The spectra were collected over the range 4000–400 cm⁻¹ by averaging 500 scans at a maximum resolution of 20 cm⁻¹ as shown in Fig 2. In case of the polycrystalline samples, scattering due to crystalline is responsible for the broad background with some asymmetric peaks. KBr reduces the quality of the spectrum below 420cm⁻¹, and hence not recorded. The 8-HQ shows intense lines above 700 cm^{-1} .

Thus it is clear that for Ca⁺⁺ doped Alq₃ the region above 749.7cm⁻¹ is dominated by the hydroxyl quinoline ligand vibrations, whereas below 648.10 cm⁻¹ the central part around the Al-atom becomes more important. In the range of 4000-2000, the broad peak at 3401.09 reveals the presence of alcohols while peak at 1604.04 and 1580.65 reveals C=O group in the synthesized complex. The absorption bands in the finger print region (1500-1400 cm⁻¹) are generally due to intra molecular phenomena, and are highly specific for each material. The peak at 1499.28 predicts aromatic ring stretching, revealing the presence of C=C group. Strong peak at 1384.95 predicts aromatic ring stretching and the presence of nitro compounds. The peak at 1329.07 reveals C-N Amines. The presence of C-O is revealed by the peak at 1115.69.The peaks between the range 1000 -400 reveals the bending of phenyl group. Two prominent peaks in the lower range at 749. 7 and 648.10 are due to C-H alkaline bonding. These results confirm the completion of quinoline ring formation and presence of quinoline structure in the metal complex.



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4. Conclusion

From the result, it concludes that the phosphor Ca^{++} doped Alq₃ prepared by low cost conventional co-precipitation method. Crystal structure is confirmed by X-Ray diffractogram method. FT-IR is an analytical technique which confirms the molecular structures of the synthesized complexes. FT-IR results confirm the completion of quinoline ring formation and presence of quinoline structure in the metal complex. Thus, prepared phosphors can be a suitable candidate in ultraviolet visible region leaving the blue and green light to be transmitted for emitting OLED, PLLCD, solid state lighting applications and ultrasound applications.

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