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LIGAND FREE SYNTHESIS AND SPECTRAL INVESTIGATION OF MONODISPERSE $CsPbBr_3$ PEROVSKITE QUANTUM DOTS

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ABSTRACT

In recent years, metal halide perovskite-structured materials have attracted the fascination of many researchers due to their unique properties and widely used optoelectronics. Defect tolerance properties of perovskite quantum dots (QDs) make them superior to conventional QDs (e.g., CdTe, ZnS, etc.). Here, we report a ligand-free, highly effective method for the preparation of highly luminescent and stable $CsPbBr_3$ perovskite via precipitation using starting materials CsBr and $PbBr_2$ in the solvent dimethyl sulfoxide (DMSO). Subsequent treatment with toluene and acetonitrile (ACN) leads to the formation of highly luminescent and more stable perovskite QDs. The stability of monodisperse CsPbBr3, crystal structure, and photophysical properties were explored using spectral analysis methods. Decomposition routes leading to nonfluorescent phases were discussed. Diffuse reflectance studies showed that perovskite QDs have a bandgap energy of 2.24 eV. Thorough crystal structure analysis confirmed that the obtained $CsPbBr_3$ perovskite QDs possess a cubic structure. This work aligns with SDG 7 – Affordable and Clean Energy.

Keywords: $CsPbBr_3$, Crystal, Diffraction, QDs, Precursor, Perovskite.

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INTRODUCTION

Metal halide perovskites (MHPs) are widely used as a new class of semiconductors for next-generation optoelectronic devices (photovoltaics[1,2], light-emitting diodes[3,4], high-energy radiation detectors[5], sensors 6, solar cells[7,8], and photodetectors[9,10] which are prepared using wet chemistry. Achieving SDG 7, which is "Affordable and Clean Energy", requires a rapid lineup of low-cost, high-efficiency photovoltaic technologies, including nanosized materials. Perovskite QDs have emerged as promising candidates due to their unique photophysical and photochemical properties and have found their niche in this field. Most inorganic lead halide perovskites, $CsPbX_3$ (where X = Cl^-, Br^-, I^-), show long-term environmental stability, and they have gradually attracted the attention of many researchers. This is especially evident in the case of the $CsPbBr_3$ structural perovskite.[11-13] There are several methods for growing $CsPbBr_3$ single crystals. These include the Bridgman method[14], the solution temperature lowering method[15], inverse temperature crystallization[16], antisolvent vapour crystallisation[17] and cooling crystallisation[18], which are widely used. In one study, a saturated standard precursor solution was prepared in the presence of DMSO and choline bromide (CB) to grow perovskite crystals with the $CsPbBr_3$ structure.

The precursor was prepared at 80 °C for 5–10 h to ensure good solubility of CsBr and $PbBr_2$ salts. To grow $CsPbBr_3$ seed crystals, a saturated solution of perovskite dissolved in DMSO was heated to 85 °C by altering the temperature from 80 °C to 85 °C by 1 °C every hour, and the process was carried out in a manner that did not allow rapid evaporation of DMSO. The development of a monodisperse single crystal of $CsPbBr_3$ was reported after 120-170 hours.[19] Common methods for synthesizing perovskite quantum dots include the ligand-assisted reprecipitation (LARP) method, which occurs at room temperature, and

the hot injection (HI) method, where heat treatment is an essential part. In a particular study to synthesise $CsPbBr_3$ quantum dots by the LARP method, precursors were prepared by first taking appropriate amounts of CsBr and $PbBr_2$ salts and dissolving them in DMSO. Oleic acid- $CH_3(CH_2)CHCH(CH_2)COOH$ (OA) and oleylamine – $CH_3(CH_2)CHCH(CH_2)_7CH_2NH_2$ (OAm) were used to control the development and size of the quantum dots as ligands. The resulting solution was added to an antisolvent to form perovskite quantum dots, and purified by centrifugation to obtain bright green fluorescent $CsPbBr_3$ quantum dots.[20] In another study, dimethylformamide (DMF) was used as a solvent to synthesise $CsPbBr_3$ perovskite quantum dots by the LARP method. CsBr and $PbBr_2$ salts were dissolved in DMF in separate vessels and mixed with OA and OLA as ligands while heating to 80 °C in a magnetic stirrer. A certain amount of the resulting precursor was taken and added to toluene under vigorous stirring in a magnetic stirrer, and green fluorescent perovskite quantum dots were formed.[21,22] The synthesis of $CsPbBr_3$ perovskite quantum dots by the hot injection route primarily requires high temperature (heating) and an inert atmosphere.

In one study, first, Cs_2CO_3 and oleic acid were dissolved in 10 ml of octadecene and mixed in a magnetic stirrer to prepare the Cs-oleate precursor. The temperature was raised to 120°C under vacuum, and an inert atmosphere was kept using nitrogen gas. Then, the $PbBr_2$ precursor was also prepared using the octadecene solvent under high temperature and an inert atmosphere. OA and OAm were added to the Pb precursor as ligands. To prepare $CsPbBr_3$ quantum dots, a certain amount of the Cs-oleate precursor was taken and added to the Pb precursor in a mixed state.

Then, the solution stirred at high temperature was rapidly cooled in an ice bath to form a lemon-colored quantum dot solution and purified.[23] In this report, highly luminescent and more stable $CsPbBr_3$ perovskite QDs were prepared. Unlike other methods where several ligands are used in the LARP route, here, no ligands were employed. Treatment with ACN induced precipitate formation. The obtained materials were investigated using a range of spectral methods.

EXPERIMENTAL

Caesium Bromide (CsBr, 99,9%), lead(II) bromide ($PbBr_2$, 99.9%), dimethyl sulfoxide ($(CH_3)_2SO$, 99.5%), toluene (C_7H_8, 99.5%), and acetonitrile (CH_3CN, 99.9%) were procured from Jinan Future Chemical Co., LTD (PR of China). All chemicals were used as obtained. UV-vis absorption spectra were acquired on a double-beam in space spectrophotometer Shimadzu UV-2600i (Shimadzu, Japan). Standard quartz cuvettes were used throughout absorption measurements. Integrated sphere UV-2600 used to obtain diffuse reflectance data from $CsPbBr_3$ perovskite QD powder. Room temperature fluorescence excitation and emission spectra were obtained on a Shimadzu RF6000 spectrophotofluorometer (Shimadzu, Japan). Diffraction patterns recorded on Shimadzu Maxima XRD 7000 (Shimadzu, Japan). A monochromatic Kα beam was used from the copper anode with a wavelength of 1.54 Å. Element composition was acquired using a NexDE VS energy dispersive spectrometer (Rigaku, Japan).

Preparation of Precursor Solution

To synthesise monodisperse $CsPbBr_3$ perovskite QDs, a modified LARP method was followed.[24] Briefly, to obtain the precursor solution, CsBr and $PbBr_2$ salts were weighed in a 1:1 molar ratio (CsBr 0.213 g and $PbBr_2$ 0.367 g). The salts were dissolved in 2 mL of DMSO and stirred on a magnetic stirrer at a temperature of 60 °C for 36 hours. The goal of this process was to attain a 0.5 M precursor solution. After 36 hours, the formation of an undissolved layer was observed in the container because of the limited solubility of the salts at the same temperature. The clear precursor solution was separated by decanting and consequently stirred for 2 hours to obtain a homogeneous medium.

Preparation of Small $CsPbBr_3$ QDs

The resultant clear precursor solution was added slowly to 5 ml of toluene under intense stirring. When the resulting toluene solution was added to 3 ml of acetonitrile, a yellow lemon precipitate was formed. The precipitate was separated, and an intense green fluorescence was observed under UV light. This yellow lemon precipitate was dried in a drying oven at 190 °C for 30 minutes, and small crystals were collected as a powder (Fig.-1).

RESULTS AND DISCUSSION

In studying the stability of $CsPbBr_3$ single crystals in humid and atmospheric environments, the structural changes of $CsPbBr_3$ perovskite QDs after their interaction with water were analyzed based on X-ray diffraction and Raman spectra.

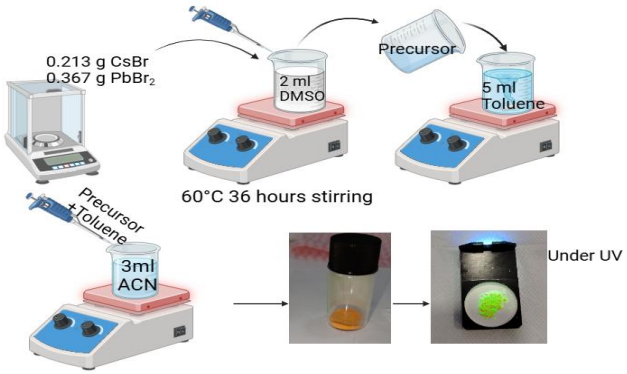

Fig.-1: Preparation of Crystalline $CsPbBr_3$ Perovskite Powder

After dehydration of $CsPbBr_3$ in humid and atmospheric environments, a decrease in its characteristic peaks (23.35º, 29.35º, 33.34º, 35.44º, 37.90º, and 47.86º) was observed. The decomposition reaction of the $CsPbBr_3$ crystal in an aqueous environment is as follows:

$$2CsPbBr_3 + H_2O \rightarrow CsBr + CsPb_2Br_5 + H_2O \quad (1)$$
$$CsPb_2Br_5 + H_2O \rightarrow CsBr + 2PbBr_2 + H_2O \quad (2)$$
$$PbBr_2 + H_2O \rightarrow PbBr(OH)\downarrow + HBr \quad (3)$$
$$PbBr(OH) \rightarrow PbO + HBr \quad (4)$$

During the experiment, the peak intensity of the XRD pattern at 20 °C for $CsPbBr_3$ is 30.37°, which was fairly weak at 59 °C and vanished at 90 °C. According to the analysis of the results of the thermodynamic stability study, the $CsPbBr_3$ perovskite QDs began to melt around 310 °C. It was confirmed that the $CsPbBr_3$ crystals were not suitable for use at temperatures above 310 °C.[25] The diffuse reflectance spectrum of a perovskite polycrystalline powder with a lemon-yellow $CsPbBr_3$ structure was used to resolve the band gap energy (E_g) using the Tauc method. In our study, the band gap energy (E_g) was calculated using the Kubelka-Munk (K-M) function.

$$F(R) = a = ((1-R)2)/(2R) \quad (5)$$

To assess the semiconductor nature, the direct and indirect band gap energies were calculated using the Tauc method (Fig.-2). For this, the diffuse reflectance spectrum was obtained from the dry powder. The indirect band gap energy was calculated using the equation $E=(\alpha hv)^{1/2}$ and extrapolated to an energy level of 2.24 eV (Fig.-3).

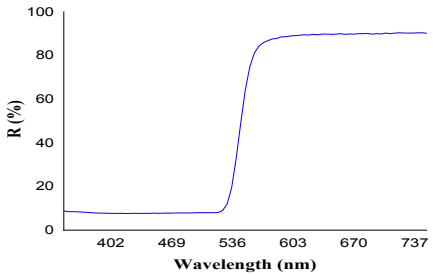

Fig.-2: Diffuse Reflectance Spectrum of $CsPbBr_3$ Perovskite Powder

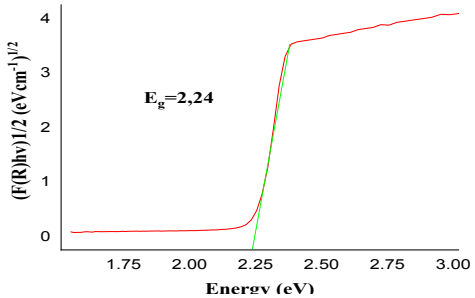

Fig.-3: Tauc Plot of $CsPbBr_3$ Perovskite

The solution above the yellow-lemon precipitate formed during the synthesis of $CsPbBr_3$ polycrystalline powder was isolated, and its photoluminescence (PL) emission spectrum was measured. The isolated

solution exhibited a distinct emission maximum at 500 nm, corresponding to bright green fluorescence (Fig.-4). This observation confirms the development of $CsPbBr_3$ perovskite QDs in the supernatant, indicating that a fraction of the product crystallises directly in the quantum-confined size regime rather than forming bulk polycrystalline powder. The photoluminescence spectrum revealed a symmetric Gaussian emission band with a full width at half maximum characteristic of highly uniform quantum dot populations. This narrow, symmetric line shape suggests minimal size dispersion and a low density of surface trap states, which are critical factors for achieving high colour purity in optoelectronic applications. Furthermore, treatment with acetonitrile (ACN) did not degrade the spectral quality; the emission band retained its symmetric Gaussian profile post-treatment. The resilience of the optical properties upon exposure to ACN suggests that the QD surfaces are well-passivated and resistant to the coordination effects of the solvent, which might otherwise induce aggregation or surface defects. The retention of the bright green emission at 500 nm after ACN treatment also implies that the quantum dots maintain their structural integrity and do not undergo significant Ostwald ripening or dissolution.

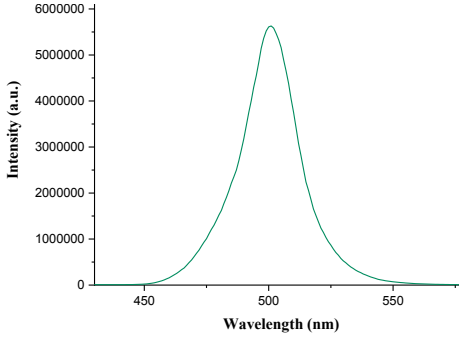

Fig.-4: Room Temperature Steady State Emission Spectrum of $CsPbBr_3$

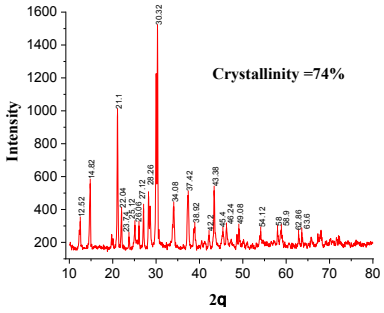

Fig.-5: XRD Spectrum of $CsPbBr_3$ Perovskite Powder Including *d* Values

The X-ray diffraction spectrum of $CsPbBr_3$ perovskite QDs exhibits peaks that indicate the crystal structure and size of the material. According to the analysis of the obtained results, it was observed that the crystal structure of the $CsPbBr_3$ containing perovskite is in the simple cubic with a space group $Pm\bar{3}m$, The degree of crystallinity of the $CsPbBr_3$ perovskite powder was found to be 74%, and the remaining 26% is amorphous or poorly crystallized (Fig.-5). The peaks in the diffraction pattern help to identify the crystal phases of the material, including its size and degree of crystallinity. The main peaks characteristic of the perovskite structure can be found in Table-1.

Table-1: Main Peak Characteristics of XRD Pattern

2θ (deg)	*hkl*	d (Å)
15.13600	(100)	5.84862
21.46900	(110)	4.13555
26.37200	(111)	3.37675
30.62200	(200)	2.92434
34.34200	(210)	2.61562
37.64100	(211)	2.38769
43.74100	(220)	2.06781
46.54500	(300)	1.94956
46.54500	(221)	1.94956
49.22500	(310)	1.84950
51.80000	(311)	1.76345
54.28800	(222)	1.68836
56.70000	(320)	1.62213
59.04700	(321)	1.56313
63.58000	(400)	1.46217
65.77900	(410)	1.41851
65.77900	(322)	1.41851

65.96300	(410)	1.41852
65.96300	(322)	1.41852
67.94100	(411)	1.37854
67.94100	(330)	1.37854
68.13300	(411)	1.37854
68.13300	(330)	1.37854
70.07000	(331)	1.34177
72.17000	(420)	1.30781
74.24700	(421)	1.27628
76.30200	(332)	1.24694

Using the FullProf software, the following Miller indices were assigned (Fig.-6). The XRD results confirmed that synthesized $CsPbBr_3$ perovskite QDs show ideal simple cubic symmetry, the space group $Pm\bar{3}m$ and the cell parameters are a = 5.84870 Å and unite cell volume 202,261991 $Å^3$ (Fig.-7).

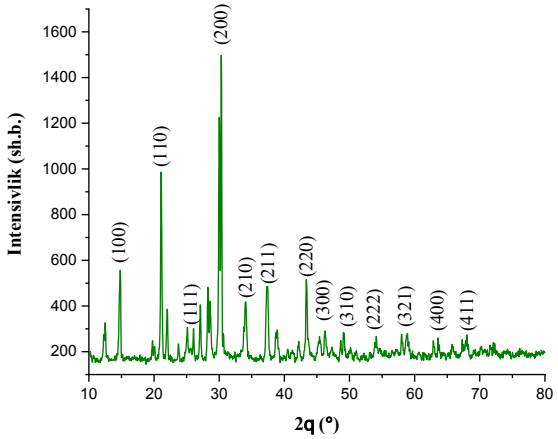

Fig.-6: XRD pattern of $CsPbI_3$ perovskite QDs

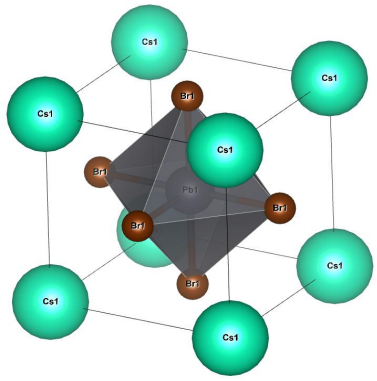

Fig.-7: Structure of $CsPbBr_3$

To evaluate the size of $CsPbBr_3$ perovskite QDs, the Scherrer method was used from the powder XRD data.

$$D = \frac{0{,}9 \cdot \lambda}{\beta \cdot \cos\theta}$$

Where D – the crystalline size (nm);

0,9 – the Scherrer constant (assuming particles have a spherical shape);

λ – the wavelength of the incident beam from the X-ray source, for the Cu anode, 1.54 Å;

β – the full width at half maximum (radian);

θ – The Bragg angle of the diffraction peak (°).

$$D = \frac{0{,}9 \cdot \lambda}{\beta \cdot \cos\theta} = \frac{0{,}9 \cdot 0{,}154\ \text{nm}}{0{,}0037 \cdot \cos 10.55} = 38{,}1\ \text{nm}$$

When analyzing the energy dispersive (ED) X-ray fluorescence spectrum of the polycrystalline sample, it was found that the mass fractions of Br (41.3%), Cs (22.9%), and Pb (35.7%) matched the $CsPbBr_3$ empirical formula. This also confirms that using ACN to precipitate perovskite QDs is suitable.

CONCLUSION

The diffuse reflectance spectrum of the $CsPbBr_3$ perovskite polycrystals was calculated to be 2.24 eV. The emission spectra were investigated to show that it was a quantum dot perovskite, i.e., the emission maximum was formed in the bright green region. It was proved that it did not lose its maximum in the bright green region even in the polycrystalline state. When analyzing energy dispersive X-ray

fluorescence spectrum of the polycrystalline sample, it was found that the mass fraction of Br (41.3%), Cs (22.9%), and Pb (35.7%) was resolved, and the structure was found to be a simple cubic. The above results also confirm the possibility of the preparation of single crystals. The proposed synthesis method may open new horizons to stable perovskite QDs.

CONFLICT OF INTEREST

The authors declare no competing financial interest.

AUTHOR CONTRIBUTIONS

The present work is related to *SDG-7: Affordable and Clean Energy*. All the authors contributed significantly to this manuscript, participated in reviewing/editing and approved the final draft for publication. The research profile of the authors can be verified from their ORCID ids, given below:

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