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Synthesis and crystal structure of bis(morpholino dithiocarbamato) Cd(II) complex and its use as precursor for CdS quantum dots using different capping agents

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ABSTRACT

Cadmium(II) morpholine dithiocarbamate complex [Cd(morphdtc)₂] was synthesized and characterized by single crystal X-ray crystallography. The molecular structure of the complex showed Cd(II) ion in a distorted 4+2 octahedral geometry, in which the two morpholine dithiocarbamates act as bidentate chelating and the central Cd ion bond the sulfur atoms of adjacent morpholine acting as bridging ligands to form centrosymmetric five coordinate dimeric molecules. The Cd(II) complex was thermolysed at 180°C to prepare CdS nanoparticles using three different capping agents. The pXRD patterns revealed a mixture of hexagonal and cubic crystalline phases of CdS nanocrystals. TEM images revealed semi-spherical and spherical nanoparticles, with the size range of 4.50-5.70 nm for OLM-CdS, 3.33-5.96 nm for HDA-CdS, and 3.00-5.83 nm for ODA-CdS. The particle size distribution of the CdS nanocrystallite is within the range 1.06 nm (SD \pm 0.73) for OLM-CdS, 0.68 nm, (SD \pm 0.73) for HDA-CdS and 1.18 nm, (SD \pm 0.60) for ODA-CdS. The lattice fringes showed that the particles are almost in the same environment with the interplanar of 0.32 nm for OLM-CdS, 0.34 nm for HDA-CdS, and 0.32 nm ODA-CdS. The band gaps energy were confirmed to be 1.59 eV for OLM-CdS, 1.65 eV for HDA-CdS, and 1.62 eV for ODA-CdS nanoparticles, respectively.

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1. Introduction

Dithiocarbamates ($R_2NCS_2^-$ or $RNHCS_2^-$) are half amides which belong to a class of monoanionic compounds known as 1,1-dithiolate that includes the dithiophosphates, dithiophosphinates, dithiocarbamates, etc. [1,2]. Dithiocarbamates are versatile ligands and bind metal ions as monodentate or bidentate chelating ligands [3,4], and have attracted interest due to their rich and varied coordination geometries [5,6]. Dithiocarbamates stabilizes transition metals with varied oxidation states and can stabilize the metal center in an extraordinarily high apparent formal oxidation states [7,8], due to vacant $d\pi$ orbitals on the sulfur atom of the dithiocarbamates moiety. They can also form multiple π -bonds and additional π -electrons which can flow from nitrogen to sulfur via a planar delocalized π -orbital system, making dithiocarbamates strong electron donors [7]. Cadmium(II) dithiocarbamate complexes continued to draw attention, due to potential industrial applications [9]. Dithiocarbamates complexes constitute one of the most promising species to provide the single-source precursor for the preparation of metal sulfidessulfides [7,10]. Single-source molecular precursor (SSP) technique has been shown to be versatile and a practical efficient route for the preparation of crystalline semiconductor (quantum dots) [11-13], which has also proven to be an effective route for better quality, crystalline monodispersed quantum dots (QDs) of semiconducting metal chalcogenide [14,15]. The use of capping agents in the preparation of quantum dots offers size stabilization and reduce reaction time [16-20]. Even though this type of technique gives a way for better control of quantum dots synthesis, quantum dots are stabilized from aggregation by addition of the capping agents as well, where the growth is hindered, resulting in high-quality form and also modify its structure, morphology and enhances their optical properties [21]. Trindade and O' Brien studied the use of cadmium dithioand diselenocarbamate complexes as precursors for the synthesis of tri-n-octylphosphine oxide/ tri-n-octylphosphine (TOPO/TOP)-capped CdS semiconductor nanoparticles [11] Ajibade et al. reported the use of Cd(II) complex of N-alkyl-N-phenyl dithiocarbamate for the synthesis hexadecylamine (HDA)-capped CdS semiconductor nanoparticles which showed rods, tripods, and tetrapods [16]. Pawar et al. themolysed nanoparticles using olevlamine/ tri-n-octylphosphine (OLM/TOP) as a capping agent and Cd(II) thiosemicarbazone which resulted in particles that are less than 10 nm in size [22]. In this study, we present the synthesis and crystal structure of Cd(II) morpholine dithiocarbamate complex and its use as a precursor to prepare CdS nanoparticles using oleylamine (OLM), hexadecylamine (HDA), and octadecylamine (ODA). The optical and structural properties of the CdS nanoparticles were studied using Ultraviolet-Visible (UV-Vis), Photoluminescence (PL), powder X-ray diffraction (pXRD) high-resolution transmission electron microscopy (HRTEM), transmission electron microscopy (TEM), scanning electron microscopy (SEM), energy dispersive X-ray spectroscopy (EDS), and Fourier Transform Infrared Spectroscopy (FTIR).

2. Experimental

2.1. Material and physical characterization

All reagents and chemicals were of analytical grade and used without further purification. Methanol, acetone, dimethyl sulfoxide, diethyl ether, morpholine, sodium hydroxide, carbon disulfide, cadmium nitrate tetrahydrate, oleic acid (OA), octadecylamine (ODA), hexadecylamine (HDA), oleylamine (OLM). FTIR spectra were recorded on a Carry 630 FTIR spectrometer using the range of 500–45,000 cm⁻¹. Bruker ultra-shield 400 NMR spectrometer was used to determine the number of protons and carbons in each compound at 400.1 MHz for 1H and 100.6 MHz for 13C nuclei. Elemental analysis was carried out using Thermo scientific Flash 2000. UV–vis spectra for the compounds were obtained from PerkinElmer Lambda UV–VIS Spectrometer. P-XRD was obtained Philips PW1830 X-Ray Diffraction Spectrometer X-ray Diffractometer (XRD). JEOL HRTEM 2100 was used for imaging and pattern diffraction of the nanoparticles. TEM images were captured using Joel 1400 Transmission Electron Microscope. SEM and EDS images were obtained from ZEISS EVO LS 15 Scanning Electron Microscope. Photoluminescence measurements were obtained from Perkin Elmer LS 45 fluorescence spectrometer. The compounds were prepared as shown in Scheme 1.

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Scheme 1. Synthesis of morpholine dithiocarbamate ligand and Cd(II) dithiocarbamate complex.

2.2. Synthesis of dithiocarbamate (DTC) ligand and its Cd(II) complex

2.2.1. Synthesis of the sodium salt of morpholine dithiocarbamate ligand

The sodium salt of morpholine DTC ligand and Cd(II) DTC complex were synthesized following a known procedure [23–26]. Sodium hydroxide (2.0 g, 0.05 mol) was dissolved in 2 mL of distilled water and allowed to attain an ice temperature. This was followed by the addition of morpholine (4.356 mL, 0.05 mol) and stirred for 5 min, after which cold carbon disulfide (3.021 mL, 0.05 mol) was added dropwise for over 5 min. The mixture was stirred for 4 h while keeping the temperature between 0°C and 4°C. The product was then filtered and washed with diethyl ether and dried under vacuum [24,27]. Yield: 8.441 g (91%), M.P: 202.3°C. FTIR (KBr, cm⁻¹): 1413 (ν C–N), 1115 (ν C = S), 939 (ν C–S). ¹H NMR (400 MHZ, D2O-*d*6): δ (ppm) = CH-protons 3.83–3.86 (t, 4H), CH-protons 4.45–4.47 (t, 4H) ppm. 13 CNMR (400 MHz, D2O-d6) δ (ppm): C_a-51.25 (C-H), C_b-65.98 (C-H), C_c-209.22 (C-N). Anal. Calc. for [C₅H₈NOS₂-]: C, 29.83; H, 4.01; N, 6.96; S, 31.85. Found: C, 29.25; H, 5.723; N, 6.94; S, 26.63.

2.2.2. Synthesis of cadmium(II)morpholine dithiocarbamate complex

Cadmium(II) morpholine dithiocarbamate complex was prepared by adding an aqueous solution of the sodium salt of morpholine dithiocarbamate (3.705 g, 0.02 mol) to an aqueous solution of $Cd(NO_3)_2 \cdot 4H_2O(2.364 \text{ g}, 0.01 \text{ mol})$, and stirred for 5 h. The precipitate was formed, filtered and washed several times with distilled water and diethyl ether then dried under vacuum [28]. Yield 5.179 g (88%), M.P: 326.6°C. FTIR (KBr, cm⁻¹): 1426 (vC-N), 980 (νC-S). ¹H NMR (400 MHZ, DMSO-*d*6): δ (ppm) = CH- protons 3.64–3.66 (t, 8H), CH- protons 4.07-4.09 (t, 8H) ppm. ¹³C NMR (400 MHz, DMSO-*d*6) δ (ppm): C_a-52.55 (C-H), C_b-66.10 (C-H), C_c-205.65 (C-N). Anal. Calc. for [C10H16CdN2O2S4]: C, 27.49; H, 3.69; N, 6.41; S, 29.35. Found: C, 27.36; H, 3.56; N, 6.32; S, 25.54.

2.2.3. X-ray crystallography

Single orange block-shaped crystals of bis(morpholino dithiocarbamato) Cd(II) complex [C₁₀H₁₆CdN₂O₂S₄] were recrystallized from DCM by slow evaporation. A suitable crystal $0.35 \times 0.18 \times 0.11$ mm was selected and mounted on a MITIGEN holder in paratone oil on a Bruker SMART APEX2 area detector diffractometer. The crystal was kept at a steady

T = 100(2) K during data collection. The structure was solved to be P21/n space group with the **ShelXS-2013** [29] structure solution program using the solution method and by using **Olex2** [30] as the graphical interface. The model was refined with version 2016/6 of **ShelXL** [30,31] using Least Squares minimization.

2.2.4. Preparation of CdS nanoparticles

Cadmium sulfide nanoparticles were prepared using the bis(morpholino dithiocarbamato) Cd(II) complex as a single-source precursor. 250 mg of the complex was dispersed in oleic acid (6 mL) as a surfactant, which was then injected into three-necked flask charged with hot octadecylamine (ODA), or hexadecylamine (HDA), or oleylamine (OLM) (3.00 g) as capping agents. The resulting mixture was refluxed for 1 h under the inert atmosphere with 400 rp, the temperature was maintained at 180°C. The product was cooled to 70°C, and about 25 mL of methanol was used to wash off excess capping agent. The resulting precipitate was separated by centrifugation at 2000 rpm for 30 min and the supernatant was discarded. The washing process was repeated thrice [22].

3. Results and discussion

3.1. Molecular structure of the Cd(II) morpholine dithiocarbamate complex

The crystallographic and measurement data depicted in Table 1 and Figure 1 shows the ellipsoid representations of the complex, respectively. Selected bond length and angles are presented in Table 2. The structure indicates that the cadmium(II) complex at 100(2)k has a monoclinic (P21/n) space group Z = 2. The planarity of the MS₂CNC₂ is the important aspect in metal dithiocarbamate complex. The complex contains Cd center with coordination sphere in which the binuclear Cd complex resides on a crystallographic inversion center and each Cd atoms is coordinated to six sulfurs atoms as a result of the Cd-S secondary bond to give the geometry around the Cd(II) ions distorted octahedral geometry [32]. The molecular structure is an unusual linear coordinated polymer of the Cd(II) where one morpholine ligand chelates one cadmium atom and simultaneously bridges the second centro symmetrically related cadmium atom, which has just been reported for a Cd(II) complex. This results in a chair conformation of the morpholine moiety.

The single crystal X-ray structure of $[C_{10}H_{16}CdN_2O_2S_4]$ showed that the Cd(II) ion is in a distorted 4 + 2 octahedral environment. The distortion of the regular octahedron geometry is mainly due to the small bite angles of the two morpholinyl dithiocarbamate ligands [32], whose S1–Cd1–S2 gives [69.467(18)] and S11–Cd1–S21 with a chelate angle of [69.468(18)], respectively. These angles deviate prominently from the normal 90° expected for a regular octahedral. The deviation produces bond angles that are different from the expected. Other Cd–S bond angles such as S21–Cd1–S1 [110.532(18)] and S2–Cd1–S11 [110.533(18)] are less than 120° which indicates that the atoms in equatorial positions. The bridging S1 atom forms the longest of the Cd–S bond lengths in the structure at 2.6213(6) Å, for the bridging bond. The Cd–S2 bond is shorter with the bond length of 2.6130(6) Å due to the double bond [33]. The C–N is the shortest bond length of 1.325(3) Å compared to the C–N bond on the ring with bond length of 1.472(3) Å due to the delocalization of the electrons in the dithiocarbamate moiety caused by the ligands bonding the Cd²⁺ ion.

Formula	$C_{10}H_{16}CdN_2O_2S_4$	
Dcalc. (g cm $^{-3}$)	2.033	
μ (mm ⁻¹)	2.112	
Formula weight	436.89	
Colour	orange	
Shape	block	
Size (mm ³)	0.35 imes 0.18 imes 0.11	
Т (К)	100(2)	
Crystal system	monoclinic	
Space group	P21/n	
<i>a</i> (Å)	4.2194(3)	
b (Å)	11.4233(8)	
<i>c</i> (Å)	14.8265(11)	
α (°)	90	
β (°)	92.955(3)	
γ (°)	90	
V (Å ³)	713.68(9)	
Ζ	2	
Ζ'	0.5	
Wavelength (Å)	0.71073	
Radiation type	ΜοΚα	
Θmin (°)	2.252	
Θmax (°)	28.436	
Measured Refl.	1796	
Independent Refl.	1796	
Reflections with $l > 2(l)$	1619	
Rint	0.0467	
Parameters	88	
Restraints	0	
Largest peak	0.563	
Deepest hole	-1.151	
GooF	1.047	
wR2 (all data)	0.0623	
wR2	0.0592	
R1 (all data)	0.0314	
R1	0.0253	

 Table 1. Summarized data of [C10H16CdN2O2S4] crystal structure.

3.2. FTIR spectral studies

FTIR spectrum of the free ligand and the metal complex were compared and assigned. Normally, FTIR spectra of dithiocarbamates compounds have three main characteristic stretching vibrations. The thioureide ν (C–N) stretching vibrations of the ligand appeared at the fingerprint region, the mode of this vibration in relation to CN stretching frequency band conformed to the fact that the bond assumes a double bond character. This band was observed at 1413 cm⁻¹ in the ligand and shifted to 1426 cm⁻¹ in the Cd(II) due to electron delocalization on the metal ion, which gives the complex higher frequency compared to that of the ligand [34]. The change in geometry has affected the extent of interaction between the DTC and the cadmium ion which resulted in the reduction of ν (C–N) stretching vibrations. The ν (C–S) which is primarily a strong band of the ligands appeared at the region of 880–915 cm⁻¹ as two bands for both asymmetric and symmetric vibrations due to the bidentate form of the ligand, and the stretching vibration band for the complex appeared at 980 cm⁻¹ as a single pronounced band. A single band in this region indicates complete symmetrical coordination of the DTC moiety to the metal center [35].



Figure 1. The molecular structure of bis(morpholino dithiocarbamato) Cd(II) complex $[C_{10}H_{16}CdN_2O_2S_4]$.

Bond length (Å)		Bond angle (°)		
Cd1–S1	2.6213(6)	S11-Cd1-S1	180.00(2)	
Cd1-S11	2.6213(6)	S2–Cd1–S11	110.533(18)	
Cd1-S21	2.6130(6)	S2–Cd1–S1	69.467(18)	
Cd1–S2	2.6130(6)	S21–Cd1–S11	69.468(18)	
S1–C1	1.745(2)	S21–Cd1–S1	110.532(18)	
S2-C1	1.724(2)	S21–Cd1–S2	180.00(2)	
N1-C1	1.325(3)	C1–S1–Cd1	85.01(8)	
N1-C2 1.474(3)	1.474(3)	C1–S2–Cd1	85.67(8)	
		C1-N1-C2	122.8(2)	
		C1-N1-C5	123.2(2)	
	C5-N1-C2	113.14(19)		

Table 2. Selected bond length (Å) and bond angle (°) of $[C_{10}H_{16}CdN_2O_2S_4]$.

3.3. Nuclear magnetic resonance (NMR) spectral studies

The ¹H NMR spectrum of morpholine dithiocarbamate ligand revealed a peak at 3.88 ppm that is due to N–CH₂. The second peak appeared at 4.45 ppm, which is for O–CH₂. The last peak is at 4.8 ppm, which is a deuterated water peak. ¹³C NMR shows NCS peak at 209.22 ppm, the second peak appeared at 65.98 ppm for O–CH₂ and the last peak appeared at 51.25 ppm for N–CH₂. In the ¹H NMR spectrum of the complex, N–CH₂ appeared as a triplet around 3.66 ppm and O–CH₂ as a triplet around 4.03 ppm, respectively. The two peaks are due to solvent, the peak at 2.52 ppm is for the solvent used for the analysis which is DMSO *d6* and the other peak at 3.26 ppm which is for the solvent used in the preparation of the complex and the solvent used analysis. ¹³C NMR revealed C–S peak at 204.65 ppm,

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N-CH₂ peak at 52.55 ppm and O-CH₂ peak at 66.10 ppm [35]. The peaks are down shifted as a result of the coordination to the metal center.

3.4. Structural studies of the CdS nanoparticles

3.4.1. Powder X-ray diffraction (pXRD) studies of CdS quantum dots

Structural identification of CdS nanoparticles was carried out using powder X-ray diffraction. The pXRD patterns of OLM, HDA, and ODA capped CdS nanoparticles are presented in Figure 2. The observed peaks are widened, which indicate that the crystallite sizes of the CdS nanoparticles are small. The diffraction patterns of the OLM-capped CdS nanoparticle corresponded to (100), (002), (101), (102), (110), (103), (112), and (203) planes which correspond to 23°, 26°, 27°, 33°, 51°, 56°, 60°, and 61°, which can be indexed to the hexagonal phase of CdS nanoparticles in the crystal system, which exactly matched with the reference code: [00-001-0780] [36]. The peaks of the HDA-capped CdS nanoparticle corresponded to (100), (002), (101), (102), (110), (103), (112), and (203) planes which corresponds to 23°, 26°, 28°, 33°, 43°, 47°, 51°, and 60°, which resembles the hexagonal structure. The XRD patterns of ODA- capped nanoparticles indicates that the (002) of the hexagonal peak is missing, thus the nanoparticles are mixture of both cubic and hexagonal structure. The pXRD peaks intensity is known to decrease and the width increases with decreasing crystalline size and there are no peaks corresponding to impurities in any of the as-prepared CdS nanoparticles [37].

3.4.2. Morphological studies (TEM) of as-prepared CdS quantum dots

TEM images, lattice fringes, and selected-area electron diffraction (SAED) patterns of OLM, HDA, and ODA-capped CdS nanoparticles are presented in Figure 3 and their particle size distributions are presented in Figure 4. The TEM image of OLM-capped CdS (Figure 3(a)) nanoparticles shows a mixture of semi-spherical and spherical particles in shapes, with uniform size distributions which range from 4.50 to 5.70 nm [38]. The lattice fringes are shown in Figure 3(b) revealed that the nanoparticles are polycrystalline, which are randomly distributed (0.90 nm) as shown in Figure 4(a) with an interplanar distance of 0.32 nm. The SAED pattern presented in Figure 3(c) denotes that the nanoparticles are polynanocrystalline in nature due to small spots making up a ring, each spot arising from Bragg reflection from an individual crystallite. CdS nanoparticles obtained from HDA-capped CdS shown in Figure 3(d) displayed close to monodispersed nanoparticles which have more particles compared to those prepared using OLM. The particles are spherical and their size ranges from 3.33 to 5.96 nm. The small size is ascribed to the quantum confinement effect, the lattice fringes in Figure 3(e) revealed that the particles are nanopolycrystalline, with a random distribution (5.250 nm) as shown in Figure 4(b) and its interplanar distance is (0.34 nm). SAED shown in Figure 3(f) displayed the diffraction pattern of nanocrystalline particles which forms a ring pattern without bright spots. There is a lot of speckle contrast blurring the contrast of the image since it has an amorphous layer at the top and bottom from the excess capping agent leading to diminishes contrast of the lattice fringes. Nanoparticles, which are displayed in Figure 3(g) containing ODA capped CdS showed little agglomeration and mixture of semi-spherical and spherical nanoparticles, it has fewer particles compared to the one of HDA capped CdS and more particles compared to the one of OLM) indicted its dom distribution (4.967 nm) as shown



Figure 2. XRD diffraction pattern of CdS nanoparticles with different capping agent.

in Figure 3(c) nanocrystalline particles with the interplanar distance of (0.32 nm). SAED in Figure 3(i) displayed well-diffracted pattern, which is due to small spots that form rings ascribed to the Bragg reflections from the individual crystallite. All the capping agent result in quantum dots with the particle size less than 10 nm.



Figure 3. TEM images, lattice fringes and SAED of OLM, HDA and ODA capped CdS nanoparticles.

3.4.3. SEM and EDS studies of the CdS nanoparticles

The Scanning Electron Microscopy (SEM) images and Energy Dispersive Spectroscopy (EDS) were employed to study morphology and elemental composition of the as-prepared



Figure 4. Size distribution of as-prepared CdS nanoparticles.

CdS nanoparticles revealed that the morphology of OLM capped nanoparticles appeared to be lumpy although it shows a smooth surface of the particles that does not have any form of arrangement. SEM micrograph of HDA capped nanoparticles shows concrete mixture like surface with different part of the particles whereas in ODA capped nanoparticles showed stone-like morphology that are composed of triangular and semi-spherical shapes, which have rough surface compared to those of OLM capped CdS. The EDS spectra of the CdS nanoparticles confirmed the elemental composition of the CdS nanocrystals as well as



Figure 5. FTIR spectra of (OLM, HDA, and ODA) capped as-prepared CdS nanoparticles.

those of the capping agents. There are an aluminum traces which displayed on the spectrum due to the sputter-coater [39].

3.4.4. FTIR spectra studies of the CdS nanoparticles

FTIR spectra of OLM, HDA and ODA cadmium sulfide nanoparticles (Figure 5). The FTIR spectra were obtained in the region between 4000 and 500 cm⁻¹. All the spectrum shown similar fatures which are ascribed to the capping agents as well as the surfactant [13]. The prominent band observed at 3336 cm⁻¹ of the nanoparticles are ascribed to v(N-H) from the capping agents (OLM, HDA, and ODA). This shows that the CdS quantum dots are capped via interaction of the $-NH_2$ group of the capping agents adsorbed on the surfaces of the nanoparticles. The absorption band observed at 2920–2853 cm⁻¹ are due to v(C-H) which arise because of the (oleic acid) surfactant used. The other important bands at 1456–1533 cm⁻¹ are attributed to v(C=O) from the carboxylic group of oleic acid (OA). The vibrational frequencies of the surfactants are in the same region with the ones of the capping agents, thus the surfactant can serve both its purpose and that of the capping agents. The significant changes observed in the fingerprint region of the nanoparticles spectra ascribed to interaction of surfactant and capping agents used. Hence the existences of the above-mentioned bands identify the presence of CdS [40].

3.5. Optical studies of CdS nanoparticles

3.5.1. Absorption and photoluminescence spectra studies of (OLM, HDA, and ODA) capped CdS nanoparticle

Optical studies of the CdS nanoparticles were investigated by means of UV–Vis and photoluminescence spectroscopy. The absorption spectra of the CdS nanoparticles presented in Figure 6(a) displayed maximum peaks at about 250 nm with the absorbance of 0.823, 0.562, and 0.551 a.u for HAD-CdS, OLM-CdS, and ODA-CdS, respectively. The absorption band edges were used to determine the band gaps energy of the CdS nanoparticles [41]. The sharp excitonic absorption peaks indicate narrow size distribution of the particles in the nanoparticles [42] The optical band gap of the cadmium sulfide nanoparticles was determined using the Tauc plot shown in Figure 6(b), which were found to be 1.59 eV



Figure 6. Absorption (a), tauc plot (b) and emission (c) spectra of cadmium sulfide nanoparticles at 180°C.

for OLM-CdS, 1.65 eV for HDA-CdS, and 1.62 eV for ODA-CdS, respectively. These were found to be blue-shifted compared to the bulk CdS [43]. The blue shift occurs due to strong quantum confinement caused by a decrease in the CdS nanoparticles of nanocrystallite size. The emission spectra Figure 6(c) displayed maxima at 421, 351, and 334 nm for ODA-CdS, HDA-CdS, and OLM-CdS, respectively. The emission maxima for ODA capped CdS was found to be higher compared to those which are obtained from HDA and OLM capped

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nanoparticles, which shows that the capping agent plays a significant role in the decomposition of the compound and the formation of the nanoparticles. The emission maxima were found to be red-shifted in comparison to the optical absorption band edges. Sizes and the increase in band gaps with the decrease in particle sizes are due to quantum confinement effects in the nanoparticles [44].

4. Conclusion

Bis(morpholino dithiocarbamato) Cd(II) complex was synthesized and characterized by single crystal X-ray crystallography, FTIR, NMR spectroscopy, and elemental analysis. The molecular structure of the compound is monoclinic with a space group of P21/n in which the compound dimerized to form a chair conformation. The bond angles of the compound denote that the molecule is 4 + 2 octahedral environment consisting of two chelating morpholine dithiocarbamate and two sulfur atoms from bridging morpholine ligands of the adjacent Cd complex. Cd(II) dithiocarbamate complex was used as singlesource precursors for CdS at 180°C using three different capping agent (OLM, HDA, and ODA). The pXRD patterns show a mixture of hexagonal and cubic crystalline phases of the CdS nanocrystals. TEM images show semi-spherical particles with the size range of (4.50-5.70 nm) for OLM-CdS, (3.33-5.96 nm) for HDA-CdS and (3.00-5.83 nm) for ODA-CdS. The lattice fringes denoted that the particles are almost in the same environment with the interplanar spacing of (0.32 nm) for OLM-CdS, (0.34 nm) for HDA-CdS and (0.32 nm) for ODA-CdS. The absorption studies of the as-prepared CdS nanoparticles showed that the edges are blue-shifted whiles the emission studies indicate that they are red-shifted due to the nanosize of the particle, the bad gaps were confirmed to be 1.59 eV for OLM-CdS, 1.65 eV for HDA-CdS, and 1.62 eV for ODA-CdS.

Supplementary materials

CCDC 1877637 contains the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data or from The Director, CCDC, 12 Union Road, Cambridge, CB2 1EZ, UK (e-mail: deposit@ccdc.cam.ac.uk).

Disclosure statement

The authors declare no conflicts of interest.

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