



Cu(II) and Ni(II) 4-cyanobenzoate complexes with nicotinamide: Synthesis, spectral, structural and optical characterization and thermal behavior

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ABSTRACT

Two new copper(II) and nickel(II) complexes $[M(\text{NC}-\text{C}_6\text{H}_4\text{COO})_2(\text{C}_6\text{H}_6\text{N}_2\text{O})_2(\text{H}_2\text{O})_2]$ (where M: Cu and Ni) have been synthesized and characterized by elemental analysis, FT-IR and UV-Vis spectroscopy, spectroscopic ellipsometer (SE), X-ray crystallography, thermal analysis and molar conductivity. X-ray measurements showed that both of the complexes crystallized in triclinic system with the space group *P*-1. The isostructure complexes have distorted octahedral geometry around the metal atom center. In both of the crystal structures, the metal atoms are coordinated by two nitrogen atoms from two different nicotinamide ligands, two carboxyl oxygen atoms from two different 4-cyanobenzoate anions and two oxygen atoms from two different water molecules. From the linear absorption spectra and spectroscopic ellipsometer measurements, it was observed that these complexes showed different optical behaviors.

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1. Introduction

Besides the cost effective synthesizing and intriguing variety of architectures depending on central metals benzoic acid derivatives are desired and investigated candidates for gas storage, ion exchange, bio-medical, luminescence, magnetic, electric properties and nonlinear optics fields [1–8]. For instance, V. Natarajan *et al.* showed that ethyl *p*-aminobenzoate had six times higher second harmonic generation (SHG) efficiency than that of potassium dihydrogen phosphate (KDP) which is well known as nonlinear optical material [7]. Metal organic frameworks (MOFs) are also suitable materials for use as functional materials in the above-mentioned applications due to their structural variability [9–15]. Metal complexes of aromatic carboxylic acids have a wide range in the literature due to their physical and biological importance as

well as different structural features. The complexes of 4-cyanobenzoic acid which is one of aromatic carboxylic acids has two different functional coordination groups exhibit structurally diversities and some physical properties due to the different ligand-metal interactions. In the literature, there are many studies on 4-cyanobenzoic acid complexes [16–21]. Over the last decade, the metal(II) arylcarboxylate complexes with ligands that containing N- and O- donor atoms have also been extensively studied because of their contributions to material science for discovering of different application fields [22–29]. Nicotinamide is also one of the N- and O- donor ligands that is usually act as a monodentate ligand by using nitrogen atom as donor of pyridine ring and rarely act as a bidentate ligand while uses both of oxygen and nitrogen atoms as donors of carbonyl group and pyridine ring, respectively. There is no complex in the literature that coordinated only with oxygen atom [28,30,31].

To the best of our knowledge, the optical characteristics (linear refraction index, linear absorption and extinction coefficients) of Cu(II) and Ni(II) arylcarboxylate complexes (complex 1 and

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complex 2, respectively) haven't been investigated in detail, yet. For this reason, in this study we investigated the optical properties of synthesized complex 1 and complex 2 by using UV–Vis spectrophotometer and spectroscopic ellipsometer (SE).

2. Experimental

2.1. Chemical reagents

The chemicals used were of reagent grade (Aldrich or Sigma) and used without further purification.

2.2. Synthesis of the complexes

2.2.1. Synthesis of diaquabis(4-cyanobenzoato- κ O)bis(nicotinamide- κ N')copper(II) (complex 1)

To prepared sodium 4-cyanobenzoate salt, 0.84 g (10 mmol) of sodium bicarbonate and 1.47 g (10 mmol) of 4-cyanobenzoic acid were mixed in 50 mL water and continuously stirred at 60 °C till removed of CO₂ gas. In another beakers, CuSO₄·5H₂O 1.24 g (5 mmol) and nicotinamide 1.22 g (10 mmol) were dissolved 50 mL water. Nicotinamide solution and sodium 4-cyanobenzoate solution were added on CuSO₄·5H₂O solution, respectively. The obtained clear solution was kept for crystallization at ambient atmosphere. After three weeks, blue single crystals that were obtained for by slow evaporation of the solution were filtered off, washed with water and dried at room temperature. Anal. Calcd. (%) for Complex 1, [Cu(NC–C₆H₄COO)₂(C₆H₆N₂O)₂(H₂O)₂] (MW = 636.08) C, 52.87; H, 4.09; N, 13.20. Found (%): C, 53.05; H, 3.80; N, 13.21; Selected IR bands (cm⁻¹): ν (OH)_{H₂O} 3500, ν (NH₂)_{arom.} 3370, ν (C–H)_{arom.} 3185, ν (C=O)_{amide} 1691, ν (C–N) 2230, ν (COO⁻)_{as} 1585, ν (COO⁻)_s 13828, $\Delta\nu$ (COO⁻) 197, ν (C–C)_{phen} 1430, δ (COO⁻) 874, δ (C–H)_{phen.} 750, ρ r(H₂O), 783 ρ w(H₂O) 652. UV–Vis [λ (nm),]: 450, 715. Molar Conductivity (μ S/cm): 5.0.

2.2.2. Synthesis of diaquabis(4-cyanobenzoato- κ O)bis(nicotinamide- κ N')nickel(II) (complex 2)

The synthesis of Complex 2 was similar to that of Complex 1 except that NiSO₄·6H₂O (1.31 g, 5 mmol) was used instead of the CuSO₄·5H₂O. After two weeks, blue single crystals that were obtained for by slow evaporation of the solution were filtered off, washed with water and dried at room temperature. Anal. Calcd. (%) for Complex 2, [Ni(NC–C₆H₄COO)₂(C₆H₆N₂O)₂(H₂O)₂] (MW = 631.22) C, 53.28; H, 3.83; N, 13.31. Found (%): C, 55.40; H, 3.56; N, 13.74; Selected IR bands (cm⁻¹): ν (OH)_{H₂O} 3173, ν (NH₂)_{arom.} 3314, ν (C–H)_{arom.} 3185, ν (C=O)_{amide} 1691, ν (C–N) 2230, ν (COO⁻)_{as} 1585, ν (COO⁻)_s 13828, $\Delta\nu$ (COO⁻) 197, ν (C–C)_{phen} 1430, δ (COO⁻) 874, δ (C–H)_{phen.} 750, ρ r(H₂O), 783 ρ w(H₂O) 652. UV–Vis [λ (nm),]: 350, 646. Molar Conductivity (μ S/cm): 8.1.

2.3. Physical measurements

Elemental analysis for C, H and N were performed by using a LECO, CHNS-932 elemental analyzer. The thermogravimetry (TG) curves were collected with a ShimadzuTG-50 analyzer. The thermal properties of the complexes were measured and recorded simultaneously with a help of Shimadzu DTG 60 thermal analyzer. The experiments were carried out in static nitrogen atmosphere with a heating rate of 10 °C min⁻¹ from room temperature to 1000 °C in platinum crucibles. The samples were approximately 10 mg and highly sintered α -Al₂O₃ was used as a reference material. The DTG sensitivity was 0.05 mg s⁻¹. Molar conductivity of the complexes were measured by using COND iSET315 in DMF (10⁻³ M) at room temperature. FT-IR Spectra were recorded on Perkin Elmer Frontier™ FT-IR Spectrometer with solid samples using a Diamond ATR

accessory in the range of 4000–600 cm⁻¹. Resolution was set up to 4 cm⁻¹, signal/noise ratio was established by 4 scans.

2.4. Crystallography

Single-crystal X-ray diffraction analyses of Complex 1 and 2 were performed on a Bruker SMART BREEZE CCD diffractometer using Mo K α (λ = 0.71073 Å) radiation at a temperature of 296 K. Structures were solved by direct methods and refined by full-matrix least squares against F² using all data [32]. All non-H atoms were refined anisotropically. Atoms H41 and H42 (for H₂O) (in Complex 1) and atoms H41, H42 (for H₂O) and H31, H32 (for NH₂) (in Complex 2) were located in difference Fourier maps and refined isotropically, while the remaining H atoms were positioned geometrically at distances of 0.93 Å (aromatic CH) (in Complex 1 and 2) and 0.86 Å (for NH₂) (in Complex 1) from the parent C and N atoms; a riding model was used during the refinement processes and the U_{iso} (H) values were constrained to be 1.2U_{eq} (carrier atom). Experimental data are given in Table 1.

2.5. Thin film deposition

For the fabrication of the thin films of all investigated complexes, 110 g/L solution of PMMA in cyclohexanone was solved in a low power sonic bath for 48 h until completely dissolved. The complex 1 and complex 2 were then added, and were also sonically agitated until they were completely dissolved and a homogeneous solution was formed. Solid-state films of samples were formed on quartz glass substrates by using a multilayer conventional spin coating technique (SCS-Spin Coat G3P). Prepared films were baked for approximately 1 h at 55 °C to facilitate the removal of residual solvent.

2.6. UV–Vis and spectroscopic ellipsometer experiments

The absorption spectra of the Complex 1 and Complex 2 films were acquired using a UV–Vis absorption spectrophotometer (Shimadzu UV-1800) versus an uncoated glass substrate as reference. SE uses to determine thicknesses and optical properties (linear refractive indices (n_0) and extinction coefficients (k)) of thin films. Work principle of ellipsometer, depends on measure the ratio of the complex Fresnel reflection coefficients, ρ , where

$$\rho = r_p/r_s = \tan \Psi \exp(i\Delta). \quad (1)$$

Ψ and Δ two parameters that are measured as angles, as result of the change of the polarization state of an incident beam is determined in reflection or transmission from linear to elliptical polarization.

SE experiments were carried out by using the instrument J.A. Woollam Co.-M2000V in the photon energy range from 1.24 to 3.34 eV (from 370 to 999 nm). All the spectra were taken at three angles of incidence (55°, 60° and 65°) to increase the fitting accuracy [33]. Optical modeling and data analysis were done using the Woollam Company WVASE32™ software package [34].

3. Result and discussion

3.1. Descriptions of the crystal structures

The X-ray structural determinations of Complex 1 and 2 confirm the assignments of their structures from spectroscopic data. Selected bond lengths and angles are given in Table 2. Hydrogen bond geometry is given in Table 3. The molecular structures along with the atom-numbering schemes are depicted in Fig. 1 and Fig. 2,

Table 1
Experimental details for Complex 1 and 2.

Compound	Complex 1	Complex 2
Empirical Formula	C ₂₈ H ₂₄ CuN ₆ O ₈	C ₂₈ H ₂₄ NiN ₆ O ₈
Colour/shape	translucent light blue/prism	translucent light blue/prism
Formula weight	636.08	631.22
Temperature (K)	296(2)	296(2)
Radiation, graphite monochr.	Mo K _α (λ = 0.71073)	Mo K _α (λ = 0.71073)
Crystal system	triclinic	triclinic
Space group	P – 1	P – 1
a, b, c (Å)	7.7563(2), 9.8735(3), 9.9911(3)	7.6441(2), 9.8583(3), 10.2482(3)
α, β, γ (°)	77.334(3), 84.430(4), 74.894(3)	78.712(3), 84.042(3), 71.740(2)
Volume (Å ³)	720.07(4)	1358.85(2)
Z	1	1
Abs. coefficients (mm ⁻¹)	0.819	0.736
D _{calc} (mg m ⁻³)	1.467	1.459
Max. crystal dim. (mm)	0.17X0.36X0.47	0.24X0.29X0.48
Θ(max) (°)	28.54	28.44
Reflections measured	3599	3591
Range of h, k, l	-10 < h < 10, -13 < k < 13, -12 < l < 13	-10 < h < 10, -13 < k < 12, -13 < l < 13
Diffractometer/scan	Bruker SMART BREEZE CCD/phi and w	
No of reflections with I > 2 σ(I)	3145	3475
Corrections applied	Lorentz polarization	
Computer programs	SHELXS-97, SHELXL-97, ORTEP-3 [32,36]	
Source of scatter. Factors	International Table for X-Ray Crystallography [37]	
Structure solution	Direct methods	
Treatment of hydrogen atoms	Geometric calculation and difference Fourier map	
No of parameters varied	204	212
GOF	1.120	1.058
R = F _o - F _c / F _o	0.0469	0.0275
R _w	0.1220	0.0763
(Δρ) _{max} (e Å ⁻³)	1.198	0.298
(Δρ) _{min} (e Å ⁻³)	-0.346	-0.243

Table 2
Selected bond lengths (Å) and angles (°) for 1 and 2.

	1	2	
Cu1–O2	1.9830(16)	Ni1–O2	2.0633(9)
Cu1–O4	2.4600(22)	Ni1–O4	2.0955(9)
Cu1–N2	2.0124(19)	Ni1–N2	2.0849(10)
O1–C1	1.239(3)	O1–C1	1.2557(16)
O2–C1	1.261(3)	O2–C1	1.2547(15)
O3–C14	1.230(3)	O3–C14	1.2356(17)
N1–C8	1.131(5)	N1–C8	1.134(3)
N3–C14	1.325(3)	N3–C14	1.3207(18)
O2–Cu1–N2	89.48(8)	O2–Ni1–N2	89.93(4)
O2–Cu1–N2 ⁱ	90.52(8)	O2–Ni1–N2 ⁱⁱ	90.07(4)
O2–Cu1–O4	94.48(8)	O2–Ni1–O4	86.97(4)
O2–Cu1–O4 ⁱ	85.52(8)	O2–Ni1–O4 ⁱⁱ	93.03(4)
N2–Cu1–O4	86.87(8)	N2–Ni1–O4	87.12(4)
N2–Cu1–O4 ⁱ	93.13(8)	N2–Ni1–O4 ⁱⁱ	92.88(4)
O1–C1–O2	126.7(2)	O1–C1–O2	125.91(12)

Symmetry codes: (i) 1 – x, 1 – y, – z, (ii) – x, – y, – z.

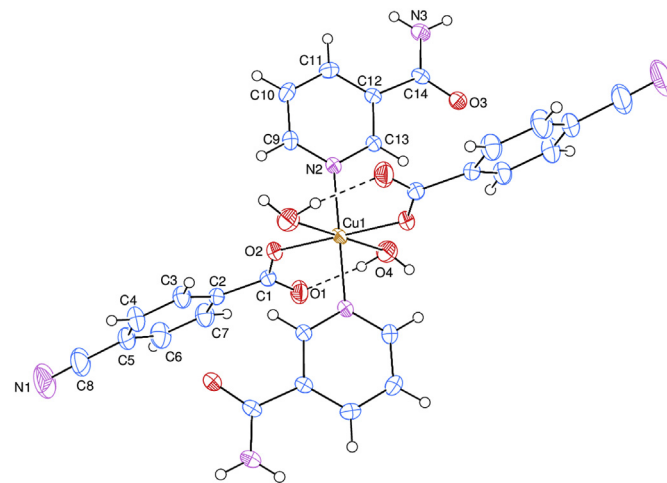
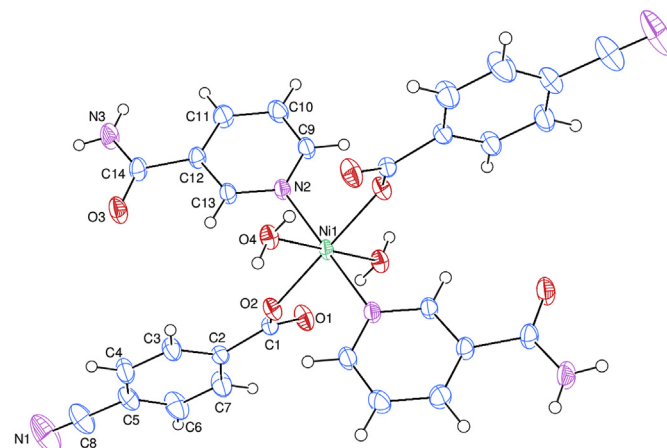
while the packing diagrams are given in Fig. 3 and Fig. 4, respectively.

In the mononuclear complexes, the metal (Cu and Ni for Complex 1 and Complex 2, respectively) atoms are located on inversion centres and coordinated by two 4-cyanobenzoate (CNB) anions, two nicotinamide (NA) ligands and two water molecules, with all ligands coordinating in a monodentate manner (Figs. 1 and 2). The two symmetry-related carboxylate O atoms (O2 and O2ⁱ) and the

Table 3
Hydrogen-bond geometry (Å, °).

Compound	D–H...A	D–H	H...A	D...A	D–H...A
1	N3–H3A...O3 ⁱ	0.86	2.07	2.885(3)	158
	N3–H3B...O1 ⁱⁱ	0.86	2.16	2.893(3)	143
	O4–H41...O3 ⁱⁱⁱ	0.80(4)	2.19(4)	2.944(3)	158(4)
	O4–H42...O1	0.88(5)	1.89(5)	2.744(3)	162(5)
	C4–H4...O1 ^{iv}	0.93	2.50	3.425(4)	171
	C9–H9...N1 ^v	0.93	2.56	3.296(6)	136
C6–H6...Cg2 ^{vi}	0.93	2.72	3.644(3)	175	
2	N3–H31...O1 ⁱ	0.85(2)	2.141(19)	2.9038(19)	149.0(19)
	N3–H32...O3 ⁱⁱ	0.83(2)	2.11(2)	2.9165(19)	165(2)
	O4–H41...O3 ⁱⁱⁱ	0.82(2)	2.12(2)	2.8844(15)	163(2)
	O4–H42...O1 ^{iv}	0.79(2)	1.85(2)	2.6460(16)	163(2)
	C4–H4...O1 ^v	0.93	2.37	3.295(2)	173
	C9–H9...N1 ^{vi}	0.93	2.55	3.298(3)	138
	C6–H6...Cg2 ^{vii}	0.93	2.76	3.6862(18)	176

Symmetry codes: [(i) 2 – x, 2 – y, 2 – z, (ii) x, 1 + y, z, (iii) 2 – x, 1 – y, 2 – z, (iv) x – 1, y, z, (v) – x, 1 – y, 1 – z, (vi) 1 – x, 1 – y, 1 – z (for 1)] and [(i) – x, 1 – y, – z, (ii) 1 – x, 1 – y, – z, (iii) 1 – x, – y, – z, (iv) – x, – y, – z, (v) 1 + x, y, z, (vi) x – 1, y, z – 1, (vii) x, 1 + y, 1 + z (for 2)]. Cg2 is the centroid of the ring (N2/C9–C13).

**Fig. 1.** An ORTEP-3 [36] view of Complex 1. The thermal ellipsoids are drawn at the 50% probability level. Hydrogen bonds are shown as dashed lines.**Fig. 2.** An ORTEP-3 [36] view of Complex 2. The thermal ellipsoids are drawn at the 50% probability level.

two symmetry-related water O atoms (O4 and O4ⁱ) form slightly distorted square-planar arrangements, while the slightly distorted

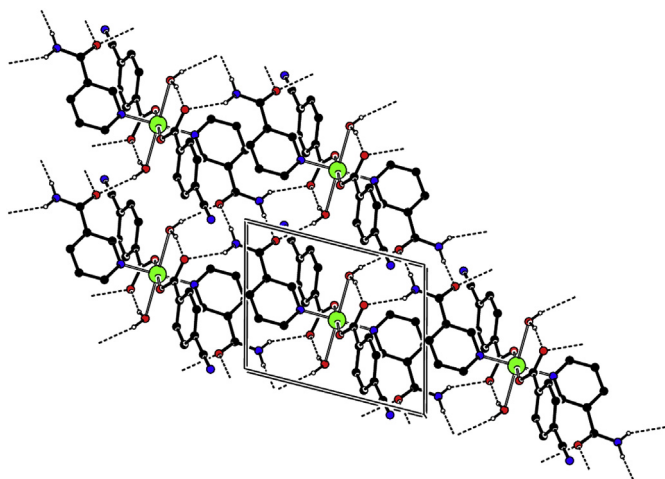


Fig. 3. A partial packing diagram of Complex 1 viewed down [001], where b-axis is horizontal and a-axis is vertical. Intermolecular N–H...O and O–H...O hydrogen bonds are shown as dashed lines. Non-bonding H atoms have been omitted for clarity.

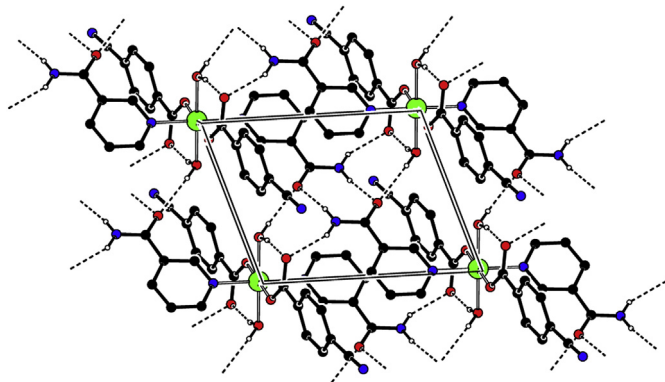


Fig. 4. A partial packing diagram of Complex 2 viewed down [001], where b-axis is horizontal and a-axis is vertical. Intermolecular N–H...O and O–H...O hydrogen bonds are shown as dashed lines. Non-bonding H atoms have been omitted for clarity.

octahedral coordination spheres are completed by the two symmetry-related N atoms (N2 and N2ⁱ) of the two NA ligands in the axial positions [symmetry codes: (i) 1 – x, 1 – y, – z (for Complex 1) and (i) – x, – y, – z (for Complex 2)]. In Complex 1, intramolecular O–H...O hydrogen bonds (Table 3) link the water hydrogens to the carboxylate oxygens.

The very similar C1–O1 and C1–O2 bond lengths (Table 2) of the carboxylate groups indicate delocalized bonding arrangements, rather than localized single and double bonds. The M – O bond lengths (where M is metal) are 1.9830(16) Å (in Complex 1) and 2.0633(9) Å (in Complex 2) (for benzoate oxygen atoms) and 2.4600(22) Å (in Complex 1) and 2.0955(9) Å (in Complex 2) (for water oxygen atoms), and the M – N bond lengths are 2.0124(19) Å (in Complex 1) and 2.0849(10) Å (in 2) (Table 2). The M atoms lie 0.4500(1) Å above (in Complex 1) and 0.3866(1) Å below (in Complex 2) the planar (O1/C1/O2) carboxylate groups. The O–M–O and O–M–N bond angles deviate only slightly from ideal values, with average values of 90(8)° (in Complex 1) and 90(4)° (in Complex 2) and 90(8)° (in Complex 1) and 90(4)° (in Complex 2), respectively (Table 2). The dihedral angles between the planar carboxylate groups (O1/C1/O2) and the adjacent benzene rings [A (C2–C7)] are 20.71(21)° (in Complex 1) and 22.30(10)° (in Complex 2), while the benzene and pyridine [B (N2/C9–C13)] rings are oriented at dihedral angles of 84.25(7)° (in 1) and 89.93(4)° (in

Complex 2).

In the crystal structures of Complex 1 and 2, N–H...O_c (c = carboxylate), N–H...O_n (n = nicotinamide) and O–H...O_n (w = water) (for Complex 1) and N–H...O_c, N–H...O_n, O–H...O_n and O–H...O_c (for Complex 2) hydrogen bonds (Table 3) link the molecules, enclosing R₂²(8) and R₄⁴(8) ring motifs [35], forming layers parallel to (001) (Figs. 3 and 4). The layers are further linked via C–H_{cnb}...O_c (cnb = 4-cyanobenzoate) and C–H_n...N_{cnb} hydrogen bonds (Table 3), resulting in three-dimensional networks. The weak C–H...π interactions are also observed (Table 3).

3.2. FT-IR spectroscopy

The absorption bands observed in the range of 3550–2900 cm^{−1} are related to the stretching vibrations of water molecules. The bands for the N–H stretches of amide group of nicotinamide appear in the range of 3438, 3437 cm^{−1}. N–H stretching vibrations for Complex 1 and Complex 2 are observed in the range of 3370–3300 and 3314–3300, respectively. The strong absorption band observed around 1670 cm^{−1} are assigned to C=O stretching vibration of carbonyl of amide group of nicotinamide. C=O stretching vibration is observed at 1691 and 1683 cm^{−1} for Complex 1 and Complex 2, respectively. Therefore, it is possible to suggest that carbonyl oxygen of nicotinamide does not participate in the coordination [28].

While nicotinamide pyridine ring vibrations are observed at 1535 cm^{−1}, those of vibrations of complexes are shifted to lower frequencies (1447 and 1448 cm^{−1}). These shifts indicate that there is coordination between the nitrogen atom of the nicotinamide ligand and the metal ion. The asymmetric (ν_{as}) and symmetric (ν_s) vibrations of the carboxylate group are observed at 1572 and 1369 cm^{−1} for Complex 1, and at 1574 and 1369 cm^{−1} for Complex 2. The Δν (ν_{as}–ν_s) values are determined as 203, 204 and 180 cm^{−1} for Complex 1 and Complex 2, respectively [16,38]. The higher Δν values compare to sodium 4-cyanobenzoate salt implies the monodentate coordination of carboxylate group. The cyano ν(C≡N) stretching vibration of the 4-cyanobenzoic acid occurs at the almost same frequency ca. 2230 cm^{−1} it is confirmed that cyano group is not involved in coordination [16,39]. FT-IR Spectra of the complexes are given in S1 and S1.

3.3. Thermogravimetric analysis

Thermal decomposition curves of the complexes are given in S3

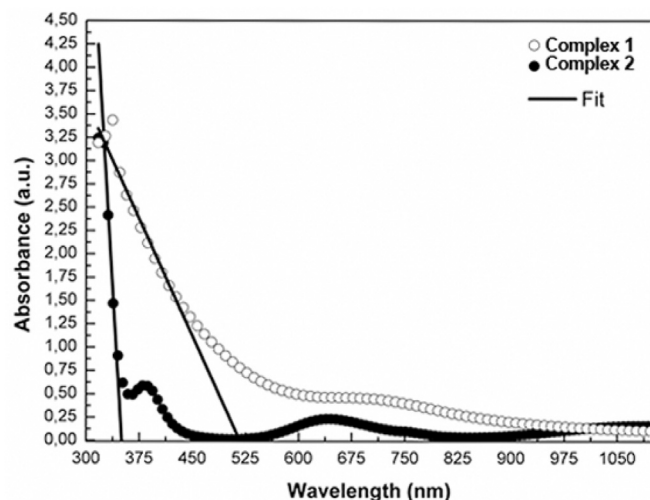


Fig. 5. Linear absorption spectra of Complex 1 and Complex 2 thin films.

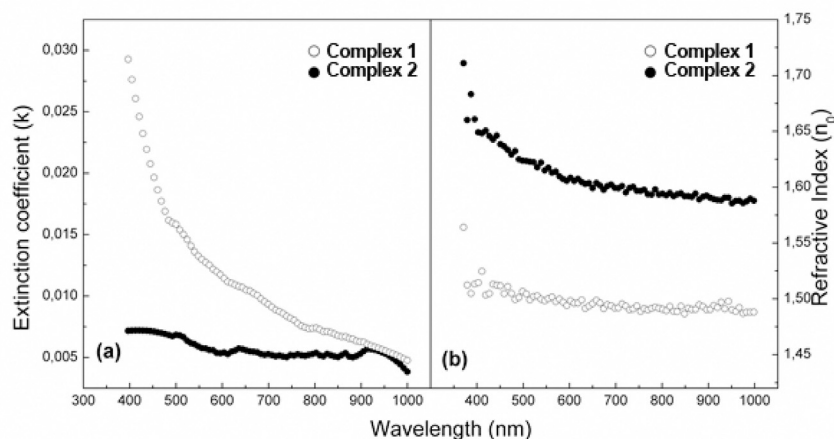


Fig. 6. The extinction coefficients and linear refractive indexes related on wavelength of the Complex 1 and Complex 2 thin films.

and S4. The complexes, Complex 1 and Complex 2, are thermally stable up to 200 °C (for 1) and 100 °C (for 2), respectively. The first stage between 225 and 250 °C (for Complex 1) and 100 and 300 °C (for Complex 2) corresponds to the endothermic elimination coordinated water molecules with a mass loss of 5.74% (calcd. 5.66%) (for Complex 1) and 5.71% (calcd. 5.74%) (for Complex 2). The continuous stages are related to release nicotinamide and 4-cyanobenzoate ligands. The thermal decomposition products are determined as CuO (for Complex 1) [87.96% (calcd. 88.17%)] and NiO (for Complex 2) [87.55% (calcd. 87.45%)], respectively [40,41].

3.4. UV–Vis absorption

The absorption spectrum provides useful information about the energy band structure and the energy gap values of studied materials. Linear absorption spectra of Complex 1 and 2 thin films are given in Fig. 5. As seen from the figure, Complex 1 and 2 are showing strong absorption behavior around 450 nm and 350 nm wavelength, respectively. This absorption behavior is consisted of sigma bands. The bands are corresponding to $\pi \rightarrow \pi^*$ transitions which involve molecular orbitals essentially are situated in the C≡N group, benzene and pyridine rings [42–45]. In addition, Complex 1 and 2 thin films have got absorption peaks around 715 nm and 646 nm wavelength, respectively. These absorption behaviors are originating from Q bands. The Q bands of thin film of Complex 1 is redshifted by 69 nm, when compared to thin film of Complex 2. The observed red spectral shift has been explained to be due to linear combinations of the atomic orbitals coefficients of the highest occupied molecular orbital (HOMO) [46,47]. The energy band gaps (E_g) of thin films were estimated with the help of the optical absorption spectra of complex 1 and complex 2 complexes thin films. We plotted $(\alpha)^2$ versus $(h\nu)$ to determined the band gap values of the films, where α is the absorption coefficient and $h\nu$ is the photon energy. E_g values of Complex 1 and Complex 2 thin films were found to be 2.412 eV and 3.549 eV, respectively.

3.5. Extinction coefficient and refractive index

The thicknesses of the complex 1 and complex 2 thin films were determined with help of SE as 201.63 nm and 62.83 nm, respectively. The identifying of the refractive index is very important for the design of optical materials. The extinction coefficients and linear refraction indexes related on wavelength of the thin films are given in Fig. 6(a)–(b), respectively. It can be clearly seen from the

Fig. 6(a) that extinction coefficient of complex 1 thin film is more increasing according to complex 2 thin film with decreasing wavelength. When Figs. 5 and 6 are compared, it can be clearly seen that the increasing of the extinction coefficient of complex 1 thin film with decreasing of the wavelength is consisted of the increasing of the refractive index rather than alteration of the absorption. As a result, the complex 1 and complex 2 thin films show different optical behaviors at same wavelengths. These discrepancies at optical behaviors can be attributed to the difference of film thicknesses and electronic properties of transition atoms, used.

4. Conclusion

In the isostructural Complexes 1 and 2, the octahedral metal atom, which rides on a crystallographic center of symmetry, is coordinated by two monodentate 4-cyanobenzoate ligands through oxygen atoms of carboxylate groups, two monodentate nicotinamide ligands through the pyridine ring nitrogen atoms and two water molecules. The band gap values of thin films of Complex 1 and Complex 2 are estimated from the linear absorption spectra as 2412 eV and 3.549 eV, respectively. In addition, from the SE measurements we observed that the refraction index and extinction coefficients of the thin films increased with decreasing wavelength. The linear absorption spectra and spectroscopic ellipsometer measurements of these complexes indicate that they are good candidates for optical filter in the ultraviolet region.

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Appendix A. Supplementary data

Supplementary data related to this article can be found at <http://dx.doi.org/10.1016/j.molstruc.2017.08.074>.

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