

Synthesis and optical properties of some isoindole-1,3-dione compounds: Optical band gap, refractive index and absorbance band edge

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Abstract: Some isoindole-1,3-dione compounds (**5**, **6**, **7**, **8**, **9**, and **10**) have been synthesized starting from 3a,4,7,7a-tetrahydroisobenzofuran-1,3-dione (**4**). Compounds **5**, **6**, **7**, **8**, **9**, and **10** were characterized by ¹H and ¹³C NMR spectra, FT-IR spectroscopy, and mass spectra measurements. The optical properties of the isoindole-1,3-dione compounds (**5**, **6**, **7**, **8**, **9**, and **10**) were also investigated. For this purpose, UV-Vis spectra of these compounds were recorded in CH₂Cl₂. The absorbance (*Abs*), transmittance (*T*), absorbance band edge (*E_{Abs-be}*), optical band gap (*E_g*), and refractive index (*n*) of these compounds were calculated and application areas of these materials were sought.

Keywords: Isoindole-1,3-dione; optical parameters; refractive index; dielectric materials; insulator/dielectric behavior. ©2018 ACG Publication. All right reserved.

1. Introduction

Norcantharimide (**1**), phthalimide (**2**), *N*-substituted norcantharimide (**3**) are some examples of isoindole derivatives containing imide (-CO-N(R)-CO-) functional group (Figure 1). These compounds and their *N*-substituted derivatives are interesting compounds due to their important biological properties in the field of synthetic organic chemistry, and medicinal chemistry.^{1,2} For this reason, many approaches have been developed for their efficient and versatile synthesis.

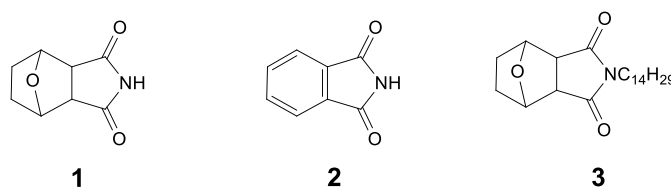


Figure 1. The structure of norcantharimide (**1**), phthalimide (**2**), and *N*-substituted norcantharimide (**3**)

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Isoindole and its *N*-substituted derivatives have received attention due to their antibacterial,² antifungal,² analgesic,² anti-HIV-1,² anxiolytic,^{2,3} anti-inflammatory,⁴ anticonvulsant,⁵ antitumor^{2,6,7,8,9} and antimicrobial activities.^{10,11} Recently, we have reported the synthesis of some isoindole derivatives and their anticancer properties.^{12,13}

Organic compounds with high nonlinear optical (NLO) properties have been used in the areas of telecommunication, high optical disk data storage, and optical information processing.^{14,15,16,17} NLO organic molecules possess delocalized π -electrons moving through the molecular system.¹⁴ Isoindoles (isoindoline-1,3-dione, isoindole-1,3-dione, and their *N*-substituted derivatives having a “-CO-N(R)-CO-” structure) are considered as eligible candidates for NLO materials because of the delocalized π -electrons. Recently, the structural, spectroscopic, and electronic properties of some *N*-substituted isoindoline-1,3-dione derivatives have been examined by both experimental and density functional theory methods.^{14,18,19,20} But the optical properties of isoindole-1,3-dione and their *N*-substituted derivatives have not been studied much.

In this study, we have reported the synthesis of novel *N*-substituted isoindole-1,3-dione derivatives (**7**, **9**, and **10**) and investigated the optical properties of compounds **5**, **6**, **7**, **8**, **9**, and **10**. We compared their optical parameters with each other. We also sought application areas for these materials.

2. Experimental

All reagents and solvents were purchased from *Sigma* and *Aldrich* without further purification. The ¹H NMR and ¹³C NMR spectra were recorded on a *Varian* 400 MHz and a *Bruker* 400 MHz spectrometer. Chemical shifts were given in parts per million (ppm). Abbreviations used to define multiplicities are as follows: *s* = singlet; *d* = doublet; *t* = triplet; *q* = quartet; *m* = multiplet. The FT-IR spectrum was recorded with a *Perkin Elmer* spectrophotometer using an ATR head in the range of 4000-600 cm⁻¹. M.p. was measured with a *Thermo Scientific* melting point device. The mass spectra were recorded on an *Agilent Technologies* 6530 Accurate-Mass Q-TOF LC/MS. Solutions and UV-Vis spectra of some isoindole-1,3-dione (**5**, **6**, **7**, **8**, **9**, and **10**) compounds: The amounts of compounds **5**, **6**, **7**, **8**, **9**, and **10** were arranged for 1 mM with a AND-GR-200 Series Analytical Balance and these compounds were dissolved in CH₂Cl₂. Then, the UV-Vis spectra of compounds **5**, **6**, **7**, **8**, **9**, and **10** were recorded with a UV-1800 *Shimadzu* model spectrophotometer at room temperature.

2.1. Synthetic procedures

2.2. General procedure for the preparation of (**5**) and (**6**) :

Ethanolamine or 1-amino-2-propanol (1 mmol) was added to a magnetically stirred solution of 3a,4,7,7a-tetrahydroisobenzofuran-1,3-dione (**4**) (1 mmol) in toluene (10 mL) and the mixture was refluxed for 36 h. The solution was cooled, diluted with EtOAc (20 mL), washed with saturated aq. NaHCO₃ (25 mL), dried with Na₂SO₄, filtered, and concentrated to give a crude product. The crude product was separated by column chromatography [(CC; SiO₂ (20 g); EtOAc/*n*-hexane, 20:80)].

2.3. *Synthesis of 2-(2-hydroxyethyl)-3a,4,7,7a-tetrahydro-1H-isoindole-1,3(2H)-dione (5)* Crystallized from CH₂Cl₂ /*n*-hexane. Yield: 95 %. Colorless crystals. M.p. 84°C. ¹H NMR (δ , ppm, 400 MHz, CDCl₃): 5.90 (*m*, 2H), 3.70 (*m*, 3H), 3.12 (*m*, 2H), 2.6 (*dm*, A part of AB system *J* = 15.0 Hz, 2H), 2.36 (*s*, OH), 2.24 (*dm*, B part of AB system, *J* = 15.0 Hz, 2H). ¹³C NMR (δ , ppm, 100 MHz, CDCl₃): 180.79, 127.73, 60.74, 41.84, 39.12, 23.52. FT-IR (cm⁻¹): 3506.19 ν (OH), 2946.67 ν (C=C-H and C-C-H), 1766.78 ν (C=O imide, asymmetric), 1670.8 ν (C=O imide, symmetric), 1410.15 ν (C=C). HR-ESI-MS: *m/z* 196.0994 [*M* + H]⁺ (calcd. 196.0968 [*M* + H]⁺)

2.4. *Synthesis of 2-(2-hydroxypropyl)-3a,4,7,7a-tetrahydro-1H-isoindole-1,3(2H)-dione (6)* was synthesized as described in our previous study.¹³

2.5. General procedure for the preparation of (7) and (8) :

To a stirred solution of (5) or (6) (1 mmol) in 10 mL of CH₂Cl₂ was added methanesulfonyl chloride (2 mmol) at 0 °C. Et₃N (2 mmol) was then added to the mixture. The mixture was stirred for 24 h at 25 °C and extracted with H₂O (3-4 × 10 mL), then dried with Na₂SO₄. The solution was evaporated under reduced pressure and gave a crude product. The crude product was separated by column chromatography [(CC; SiO₂ (25 g); EtOAc/*n*-hexane, 20:80)].

2.6. *Synthesis of 2-(1,3-dioxo-3a,4,7,7a-tetrahydro-1H-isoindol-2(3H)-yl) ethylmethanesulfonate (7)* Crystallized from CH₂Cl₂/*n*-hexane. Yield: 98 %. Colorless crystals. M.p. 82 °C. ¹H NMR (δ, ppm, 400 MHz, CDCl₃): 5.90 (*m*, 2H), 4.36 (A₂ part of A₂B₂, 2H), 3.80 (B₂ part of A₂B₂, 2H), 3.13 (*m*, 2H), 3.01 (*m*, 3H), 2.59 (*dm*, A part of AB, *J* = 15.3 Hz, 2H), 2.24 (*dm*, B part of AB, *J* = 15.3 Hz, 2H). ¹³C NMR (δ, ppm, 100 MHz, CDCl₃): 179.8, 127.8, 64.8, 39.1, 38.0, 23.4. FT-IR (cm⁻¹): 3025.0-2955.31 ν(C=C-H and C-C-H), 1762.80 ν(C=O imide, asymmetric), 1688.44 ν(C=O imide, symmetric), 1414.05 ν(C=C).

HR-ESI-MS: *m/z* 274.0772 [*M* + H]⁺ (calcd. 274.0743 [*M* + H]⁺)

2.7. *Synthesis of 1-(1,3-dioxo-3a,4,7,7a-tetrahydro-1H-isoindol-2(3H)-yl)propan-2-yl methanesulfonate (8)* was synthesized as described in our previous study.¹³

2.8. General procedure for the preparation of (9) and (10) :

To a stirred solution of (7) or (8) (1 mmol) in 10 mL of DMF was added NaN₃ (3 mmol) at room temperature. Ambient temperature was fixed at 70 °C and the mixture was stirred for 24 h. The solution was evaporated under reduced pressure. To the mixture was added 10 mL of CH₂Cl₂ and extraction was performed with H₂O (2 × 10 mL), followed by drying with Na₂SO₄ to give a crude product. The crude product was separated by column chromatography [(CC; SiO₂ (20 g); EtOAc/*n*-hexane, 10:90)].

2.9. *Synthesis of 2-(2-azidoethyl)-3a,4,7,7a-tetrahydro-1H-isoindole-1,3(2H)-dione (9)* Yield: 87 %. Crystallized from CH₂Cl₂/*n*-hexane. Yellow crystals. M.p. 80°C . ¹H NMR (δ, ppm, 400 MHz, CDCl₃): 5.90 (*m*, 2H), 3.67 (A₂ part of A₂B₂, 2H), 3.45 (B₂ part of A₂B₂, 2H), 3.10 (*m*, 2H), 2.62 (*dm*, A part of AB, *J* = 10.9 Hz, 2H), 2.24 (*dm*, B part of AB system, *J* = 10.9 Hz, 2H). ¹³C NMR (δ, ppm, 100 MHz, CDCl₃): 179.8, 127.7, 48.2, 39.1, 37.8, 23.5. FT-IR (cm⁻¹): 2953.57-2850.00 ν(C=C-H and C-C-H), 2128.94 ν(N=N=N), 2095.64 ν(N=N=N), 1769.93 ν(C=O imide, asymmetric) , 1691.46 ν(C=O imide, symmetric), 1426.54 ν(C=C).

HR-ESI-MS: *m/z* 221.1096 [*M* + H]⁺ (calcd. 221.1039 [*M* + H]⁺)

2.10. *Synthesis of 2-(2-azidopropyl)-3a,4,7,7a-tetrahydro-1H-isoindole-1,3(2H)-dione (10)* Crystallized from CH₂Cl₂/*n*-hexane. Yield: 80 %. Light yellow crystals. M.p. 39-40°C. ¹H NMR (δ, ppm, 400 MHz, CDCl₃): 5.90 (*m*, 2H), 3.78 (*m*, 1H), 3.57 (*dd*, A part of AB system, *J* = 13.4, 8.5 Hz, 1H), 3.4 (*dd*, B part of AB, *J* = 13.4, 5.0 Hz, 1H), 3.11 (*m*, 2H), 2.62 (*dm*, A part of AB system, *J* = 14.5 Hz, 2H), 2.24 (*dm*, B part of AB, *J* = 11.8 Hz, 2H), 1.24 (*d*, *J* = 6.6 Hz, 3H). ¹³C NMR (δ, ppm, 100 MHz, CDCl₃): 179.91 (179.89), 127.80 (127.70), 54.93, 43.82, 39.08 (39.04), 23.57 (23.50), 17.18. FT-IR (cm⁻¹): 2970.68-2800.00 ν(C=C-H and C-C-H), 2104.21 ν(N=N=N), 1769.93 ν(C=O imide, asymmetric), 1691.46 ν(C=O imide, symmetric), 1429.18 ν(C=C).

HR-ESI-MS: *m/z* 235.1203 [*M* + H]⁺ (calcd. 235.1195 [*M* + H]⁺)

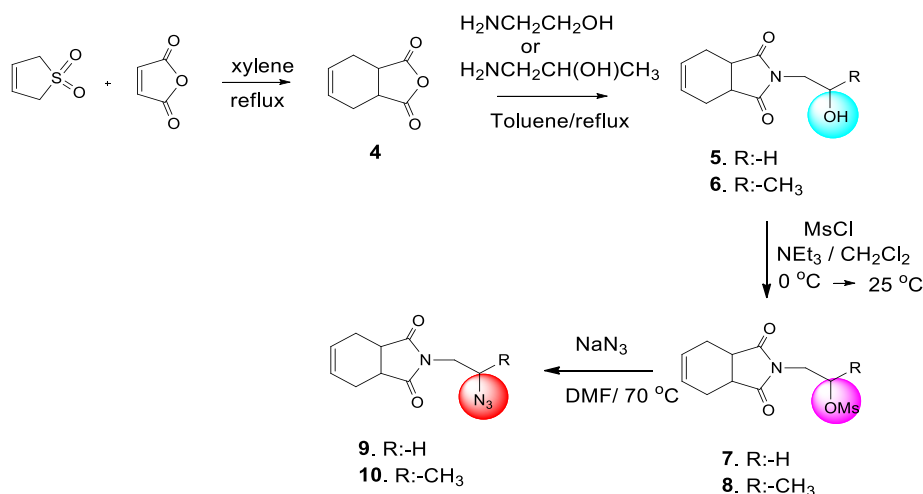
3. Result and Discussion

3.1. Synthesis

Compounds 5-10 were synthesized starting from 3a,4,7,7a-tetrahydroisobenzofuran-1,3-dione (4). Compounds 4, 6, and 8 were synthesized as described in our previous studies^{13,21} and compound 5 is

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known in the literature.²² Compounds **7**, **9**, and **10** are novel *N*-substituted isoindole-1,3-dione derivatives. The synthesis of all compounds was performed in three stages. For this purpose, first, the condensation of ethanolamine or 1-amino-2-propanol with compound **4** in toluene was carried out to synthesize imide compounds **5** and **6** as in our previous work (Scheme 1).^{13,21}



Scheme 1. The synthesis of imide compounds **5**, **6**, **7**, **8**, **9**, and **10**.

Imide compounds **5** and **6** were subjected to methanesulfonyl chloride for 24 h at temperatures from 0 °C to room temperature in dichloromethane to obtain compounds **7** and **8** (Scheme 1). Compounds **9** and **10** were synthesized via substitution of compounds **7** and **8** with NaN₃ for 24 h at 70 °C in *N,N*-dimethylformamide (DMF). “-OMs” group was replaced with azide “-N₃” group having delocalized π -electrons. The structures of compounds **9** and **10** were assigned by the ¹H NMR, ¹³C NMR, and FT-IR spectra.

3.2. Optical properties

The UV-spectrum of a material can be analyzed with absorbance (*Abs*), transmittance (*T*), and reflectance (*R*) measurements. Figure 2a indicates the absorbance curves versus the wavelength (λ) of compounds **5**, **6**, **7**, **8**, **9**, and **10**. As seen in Figure 2a, compounds **5**, **6**, **7**, **8**, **9**, and **10** display maximum absorbance peaks at 229, 231, 230, 230, 229, and 229 nm, which correspond to the near ultraviolet (NUV) region.^{23,24} As seen in Figure 2a, the absorbance spectra of compounds **5**, **6**, **7**, **8**, **9**, and **10** are dominant in the NUV region, while the absorbance spectra of compounds **5**, **6**, **7**, **8**, **9**, and **10** are almost constant in the visible (V) region. It is seen that there is a difference among the absorbance spectra of compounds **5**, **6**, **7**, **8**, **9**, and **10**, but the wavelengths of their maximum absorbance peaks are almost unchanged.

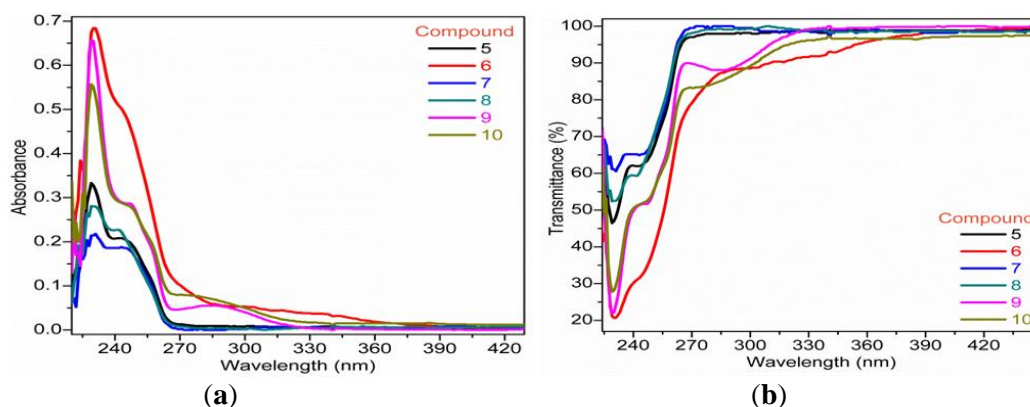


Figure 2. The (a) absorbance and (b) transmittance curves vs. wavelength (λ) of compounds **5**, **6**, **7**, **8**, **9**, and **10**.

Figure 2b indicates the transmittance curves versus λ of compounds **5**, **6**, **7**, **8**, **9**, and **10**. These compounds have very high permeability. The transmittance spectra of compounds **5**, **6**, **7**, **8**, **9**, and **10** are dominant in V region.

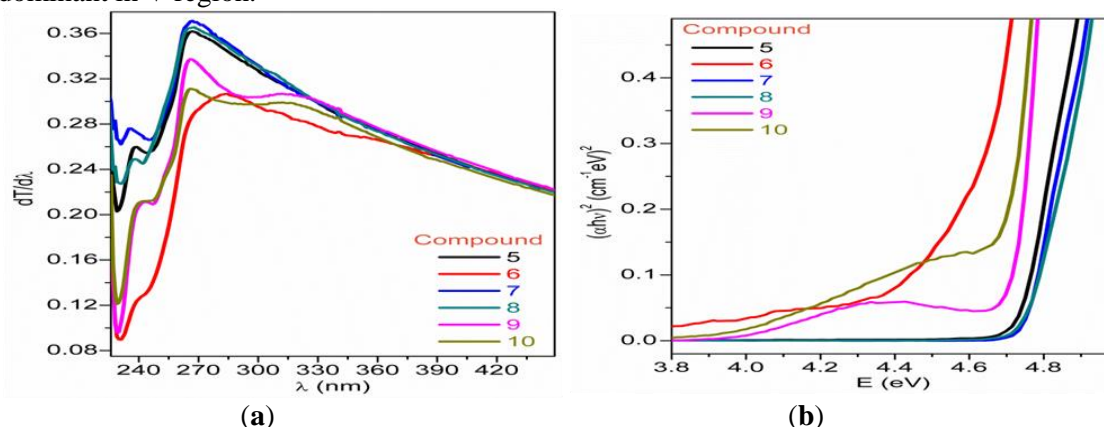


Figure 3. The (a) $dT/d\lambda$ curves versus λ and (b) $(\alpha h\nu)^2$ curves versus photon energy (E) of compounds **5**, **6**, **7**, **8**, **9**, and **10**.

We plotted the $dT/d\lambda$ curves versus λ of compounds **5**, **6**, **7**, **8**, **9**, and **10** as seen in Figure 3a, to obtain the absorbance band edge (E_{Abs-be}), which gives useful features for optical properties. The E_{Abs-be} values of these compounds were calculated from the maximum peaks of the curves and are given in Table 1. As seen there, the E_{Abs-be} of these compounds varies from 4.366 to 4.662 eV.

Table 1. The absorbance band edge (E_{Abs-be}) and optical band gap (E_g) of compounds **5**, **6**, **7**, **8**, **9**, and **10**.

Compounds	E_{Abs-be} (eV)	E_g (eV)
5	4.644	4.672
6	4.366	4.236
7	4.644	4.700
8	4.627	4.671
9	4.662	4.627
10	4.662	4.532

Table 2. The refractive index parameters obtained from the Moss, Herve-Vandamme, Reddy and Kumar-Singh relations of compounds **5**, **6**, **7**, **8**, **9**, and **10**.

Compounds	Refractive index (n) values			
	Moss	Herve-Vandamme	Reddy	Kumar-Singh
5	2.124	1.947	2.445	2.048
6	2.176	2.029	2.512	2.114
7	2.120	1.942	2.441	2.044
8	2.124	1.947	2.446	2.049
9	2.129	1.955	2.452	2.049
10	2.140	1.972	2.466	2.069

The optical band gap (E_g) determines the band structure and type of conductivity of the material, and is one of the most important parameters in the investigation of optical properties. To obtain the E_g values of compounds **5**, **6**, **7**, **8**, **9**, and **10**, we used the Tauc model²⁵ and benefited from its applications.^{23,24,26} For this, we plotted the $(ah\nu)^2$ curves versus photon energy (E) (α is the absorption coefficient) of these compounds as seen in Figure 3b. As shown in Table 1, the E_g value (4.236 eV) of compound **6** is the lowest, while the E_g value (4.700 eV) of compound **7** is the highest.

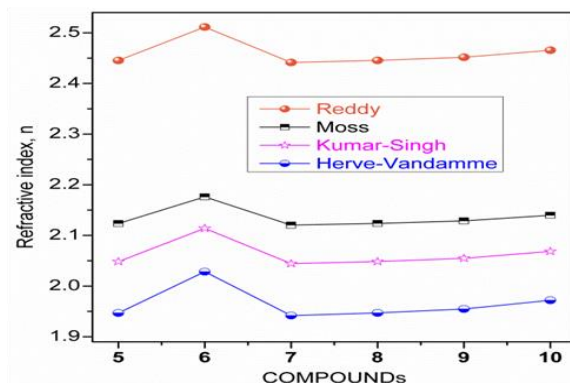


Figure 4. The refractive index curves for different compounds and relations.

The refractive index (n) has a very important place among the parameters of the optical properties and can be obtained from many different techniques and equations. The refractive indices of compounds **5**, **6**, **7**, **8**, **9**, and **10** were obtained from various relations,^{27,28} such as the Herve-Vandamme, Kumar-Singh, Moss, and Reddy relations. The obtained refractive indices of these compounds are given in Table 2. Figure 4 indicates the n curves for different compounds and relations. It is seen that the refractive index of these compounds varies from 1.942 to 2.512.

As a conclusion, this study was carried out in two stages. First, some isoindole-1,3-dione compounds (**5**, **6**, **7**, **8**, **9**, and **10**) were synthesized starting from 3a,4,7,7a-tetrahydroisobenzofuran-1,3-dione (**4**) in three stages. All compounds were synthesized by simple but effective methods. These compounds have “-OH, -OMs, and -N₃” functional groups and are very important as starting materials for substitution reactions and click chemistry. Secondly, the optical properties of these compounds were investigated by UV-Vis absorption spectroscopy and their optical parameters were compared with each other. The UV-Vis spectra of these compounds were recorded in CH₂Cl₂. The Abs , T , E_{Abs-be} , E_g , and (n) of these compounds were calculated. The Abs curves of these compounds are dominant in the NUV region and the Abs peaks vary from 229 to 231 nm. The T curves of these compounds are dominant in the V region with high permeability. Therefore, these compounds can be seen as advantageous for technologies and applications that require high permeability. The E_{Abs-be} of these compounds varies from 4.366 to 4.662 eV, indicating insulator materials with very poor conductivity. The E_g of compounds **5**, **6**, **7**, **8**, **9**, and **10** exhibit insulator/dielectric behavior and these compounds can be used as the oxide layer in metal oxide semiconductors and as insulating layers in transistors. The refractive indices of these compounds were calculated. As seen in Figure 4, the highest refractive indices are obtained from the Reddy relation for compound **6**, while the lowest refractive indices are obtained from the Herve-Vandamme relation for compound **7**. These results showed that the different functional groups (“-OH, -OMs, and -N₃”) in the molecules (**5-10**) do not significantly change their optical properties.

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Supporting Information

Supporting information accompanies this paper on <http://www.acgpubs.org/journal/organic-communications>

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