Study of the Optical Properties of Isonitrosoacetophenone ($C_8H_7NO_2$) Using UV-Vis Spectroscopy

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Abstract: In this work, the optical properties (absorption, absorption coefficient, refractive index, band- gap energy, extension coefficient, and reflection) of the five samples of isonitrosoacetophenone ($C_8H_7NO_2$) was studied using Uv-Vis spectroscopy. The $C_8H_7NO_2$ was dissolved in different amounts of (0.5, 1, 1.5, and 2) ml of distilled water. The effect of concentration on the optical properties of $C_8H_7NO_2$ was investigated experimentally and it was shown that the different values of the calculated optical properties are clearly affected by the concentrations of the $C_8H_7NO_2$ compound. In addition, when the isonitrosoacetophenone is mixed with 2.0 ml of water the absorbance rate of the pure isonitrosoacetophenone was shown to be decreased from 2.7×10^{-4} (a. u.) at 278 nm to 1×10^{-4} (a. u.) at the same wavelength. Furthermore, the transmission of $C_8H_7NO_2$ was shifted towards the shorter wavelength as the concentration of water is increased, which is starts from ~346 nm for pure isonitrosoacetophenone and decreased to ~ 300 nm when mixed with 2.0 ml of water. The important finding of this work was that the compound $C_8H_7NO_2$ is opaque (non-transmittance) material from the wavelength of 220 to 300 nm which corresponds to the UV portion of the electromagnetic spectrum and this suggests more study in this area.

Keywords: Isonitrosoacetophenone, Optical Properties, Uv-vis Spectroscopy, Band-gap Energy

1. Introduction

Isonitrosoacetophenone is one of the most promising oximes with its wide range of applications [1, 2]. Oximes are highly crystalline and are useful for purification and characterization of carbonyl compounds; it is also useful as efficient protecting groups for ketones and aldehydes [3, 4]. The isonitrosoacetophenone as the other oximes has important analytical applications in the determinations of the metal concentration from natural products. The Isonitrosoacetophenone (INAP) ligands have catalytic and biological activities. Oximes and dioxides exhibit a broad range of pharmacological activity, including antibacterial; antidepressant and antifungal. The literature survey of the past

few years reveals the fact that a significant development in the field of biological activity of metal chelates plays a vital role in the cause and treatment of cancer [4]. Structural and optical studies of the complexes of transition metals from the isonitrosoacetophenone are not carried so far. The preparation and properties of the complexes of oxime imine compounds especially the isonitrosoacetophenone is still a large area of research [5]. The chemical structure of $C_8H_7NO_2$ is shown in figure 1 with the molecular weight of 149.14700g/mol.
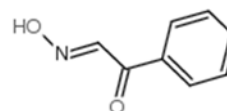

Figure 1. Chemical structure of the Isonitrosoacetophenone.

Isonitrosoacetophenone shows great interesting especially in the field of the drug design, and protein and DNA functions, the ligand-binding phenomenon plays a crucial role [5].

In this work, the optical properties (absorption, absorption coefficient, refractive index, band-gab energy, extension coefficient, and reflection) of the isonitrosoacetophenone was studied using Uv-Vis spectroscopy. The isonitrosoacetophenone ($C_8H_7NO_2$) was dissolved in different amounts (0.5, 1, 1.5, and 2) ml of distilled water and also the effect of concentration on the Isonitrosoacetophenone optical properties was investigated.

2. Materials and Methods

2.1. Materials

Distilled water, AR grade 2- Isonitrosoacetophenone (INAP) powder with the properties shown in table 1 imported from china which was used in this study.

Table 1. *The most important physical properties of the Isonitrosoacetophenone.*

Color	Beige to yellowish crystalline
Boiling Point	305.7°C at 1 atm
Melting point	122-126°C
Density	1.13 g/cm^3
Storage Temperature	2-8°C

2.2. UV-Vis Spectrometer

Uv-vis spectrophotometer model UV-mini 1240 with the most important specifications listed in the table 2 used to record the absorption, transmission, absorption coefficients, and the band gap energy of the isonitrosoacetophenone sample dissolved in different concentrations of water was manufactured by Shimadzu Japan [6].

Table 2. *The most important specifications of the UV-vis spectrometer used in this work.*

Wavelength range	190.0 to 1100.0 nm
Display wavelength	0.1 nm step
Selectable wavelength	0.1 nm step (1 nm step in spectrum mode)
Light sources	Selectable from the following 3 types; Auto change with wavelength, Selectable wavelength 295 nm to 364 nm: 1 nm interval, Recommended wavelength: 340 nm, Halogen lamp only Deuterium (D_2) lamp only
Measurement method	Single beam measurement
Monochromator	Incorporates aberration-correcting concave blazed holographic grating
Detector	Silicon photodiode
Spectrum bandwidth	5 nm
Wavelength accuracy	±1.0 nm
Stray light	less than 0.05% (220.0 nm NaI, 340.0 nm $NaNO_2$ & UV39)

2.3. Method

The procedure to complete this work was done as follows, the optical properties of the pure Isonitrosoacetophenone were measured using the UV spectrometer, then the Isonitrosoacetophenone was dissolved in distilled water with concentrations of 0.5, 1, 1.5, and 2 ml. Accordingly, the above different concentrations of Isonitrosoacetophenone compound were used to study its variation on the optical properties. Then the obtained results were plotted using the origin program and discussed in detail. In the case of band-gap energy, the value of the constant (n) was examined too, and its clear effect on the optical band gap energy was verified.

3. Results and Discussion

The optical properties of pure isonitrosoacetophenone ($C_8H_7NO_2$) and with adding different distilled water concentrations were studied using the Uv-Vis spectrometer. The absorbance of the pure isonitrosoacetophenone and that of the mixed with water at (0.5, 1.0, 1.5, and 2.0) ml concentrations against the wavelengths are shown in figure 2.

Figure 2 shows the absorbance of pure isonitrosoacetophenone and the mixed one with different concentrations of water. The mixed ones are measured at room temperature as a function of wavelengths in the spectral range from 189 nm to 400 nm. However, the pure isonitrosoacetophenone has a maximum absorbance than the mixed one. The absorbance edge of the Isonitrosoacetophenone occurs at a wavelength around (268 nm) corresponding to photon energy (4.6 eV). As shown in figure 2, the absorbance of the isonitrosoacetophenone sample decreased as the result of the increase in the concentration of water.

The transmission spectra of the isonitrosoacetophenone (pure and mixed with different concentrations of water) are shown below in figure 3.
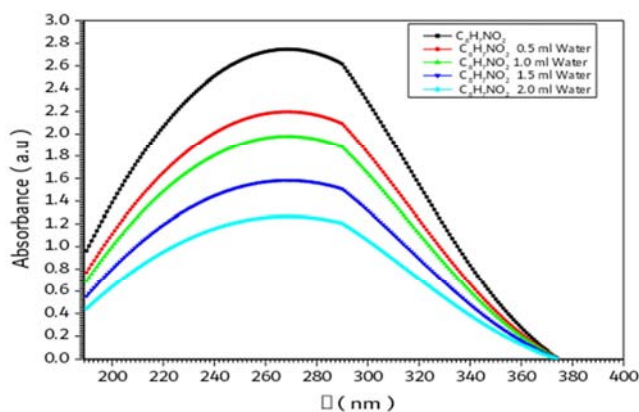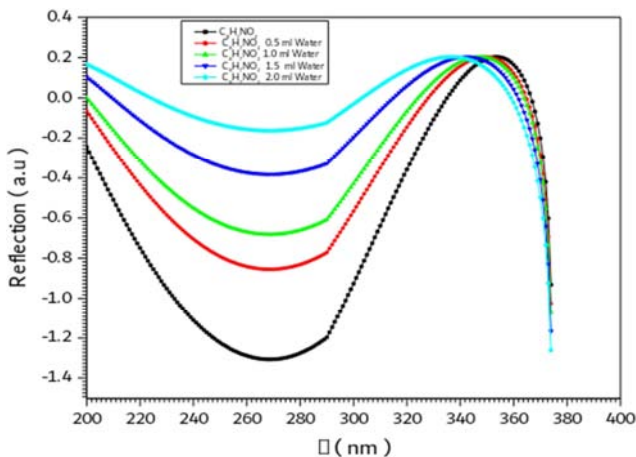

Figure 2. *Absorbance versus wavelength of isonitrosoacetophenone with and without water.*
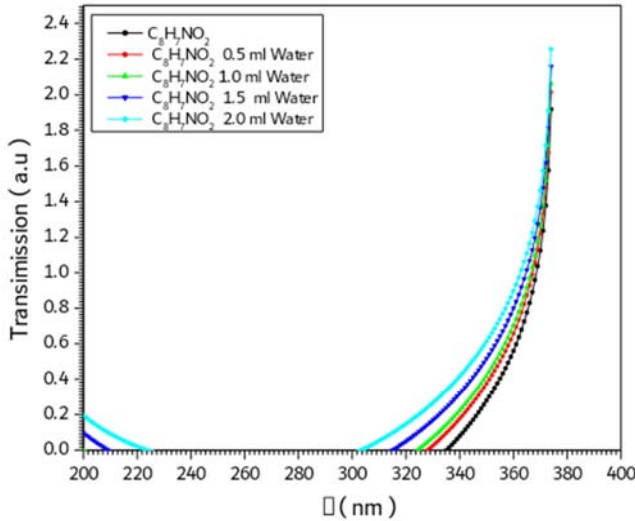
Figure 3. Transmission spectra of Isonitrosoacetophenone with and without water.

The optical transmission spectra of the pure isonitrosoacetophenone ($C_8H_7NO_2$) and of that mixed with different concentrations of water as a function of wavelengths are shown in figure 3, the transmittance spectra decrease form the wavelength 370 nm to wavelength 308 nm and the mean transmittance of all samples is 2.24 (a. u.) occurs at wavelength 370 nm. The value of transmittance for all samples decreases while the concentration of the water is increased, this concept supported the previous argument. Figure 4 shows the reflection spectra of all isonitrosoacetophenone samples.

Figure 4 shows the reflectance of isonitrosoacetophenone ($C_8H_7NO_2$) with and without water, which are measured at room temperature as a function of wavelength in the spectral range from 189 nm to 400nm. It shows the reflectance spectra, and the maximum value of (Peak of the reflectance R) for all samples which is equal (0.2 a. u) at different wavelength is ranged from (352 nm for the $C_8H_7NO_2$ without water and at 330 nm for the $C_8H_7NO_2$ when 2.0 ml of water is added. In addition, as the results are shown in figure 4 the peak is shifted towards the shorter wavelengths as a result of increasing the concentration of water.

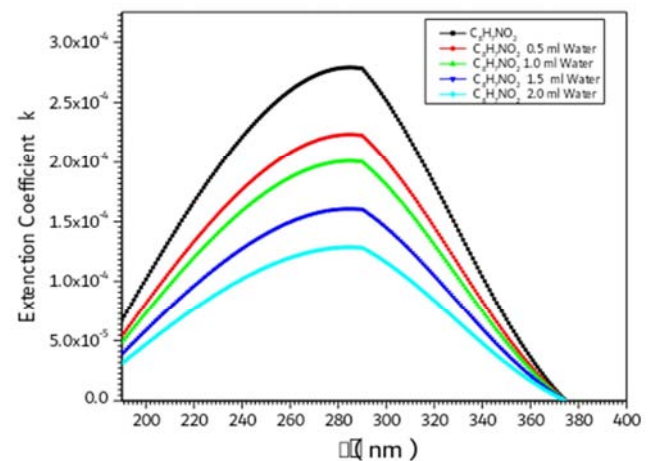*Figure 4. The reflection spectra of Isonitrosoacetophenone with and without water.*
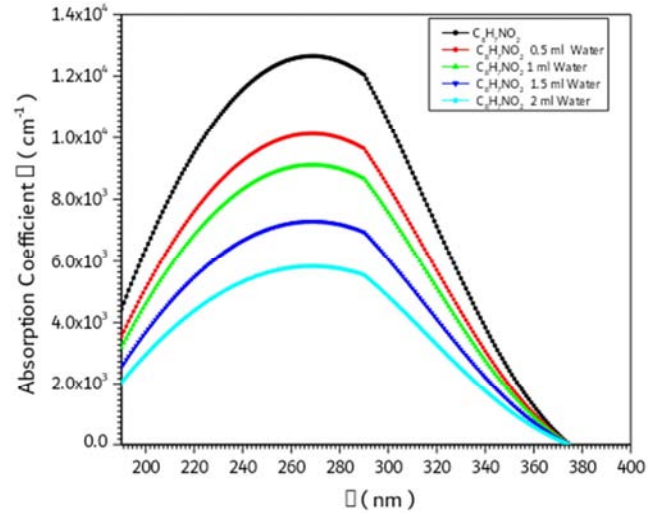
Figure 5. The absorbance's Coefficients of Isonitrosoacetophenone with and without water.

The absorption coefficient (α) of the five ($C_8H_7NO_2$) samples can be determined by the following formula [7, 8]:

$$a = \frac{2.303.a}{x} \qquad (1)$$

where (a) is the absorbance and (x) is the optical length on the samples. The plot of (α) for pure and mixed Isonitrosoacetophenone with different water concentrations versus wavelengths are presented in In Figure 5, we noticed from this figure, the large value of α $>1.28\times10^4$ cm^{-1} corresponds to the pure $C_8H_7NO_2$, which is fall in the UV region (around the 276 nm wavelength). This clearly means the transition must be corresponding to a direct electronic transition, and the properties of this state are important since they are responsible for electrical conduction. Furthermore, Figure 6 shows the extension coefficients of the isonitrosoacetophenone at different water concentrations.


Figure 6. The extension coefficients of Isonitrosoacetophenone with and without water.

Extinction coefficient (K) was calculated by the following equation [8]:

$$K = \frac{a\lambda}{4\pi} \qquad (2)$$

the variation at the (K) values as a function of (λ) is shown in figure 7, it is observed that the spectrum shape of (K) has the same shape of absorption (α) spectrum. The obtained value of (K) at the UV region where the value of (K) at (283) nm of the pure isonitrosoacetophenone is (2.79×10^{-4}) while for the mixed C$_8$H$_7$NO$_2$ with 2.0 ml water at the same wavelength is 1.28×10^{-4}, this means, the pure isonitrosoacetophenone has a large extension coefficients than the mixed with 2.0 ml one. Figure 7 shows the refractive indices versus wavelengths of the pure and mixed isonitrosoacetophenone with different concentrations of water.
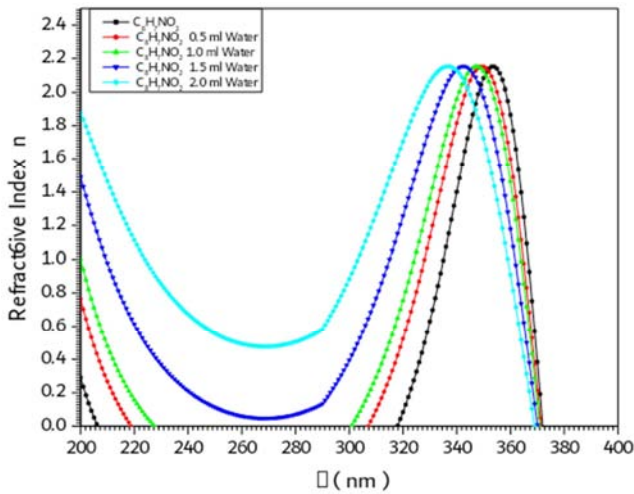
Figure 7. The refractive indices of pure and mixed Isonitrosoacetophenone with water.

The refraction index of the C$_8$H$_7$NO$_2$ samples is given by the following relation [9]:

$$n = \left[\left(\frac{1+R}{1-R}\right) - (k^2 + 1)\right]^{\frac{1}{2}} + \left(\frac{1+R}{1-R}\right) \qquad (3)$$

where (k) is the extinction coefficient which is shown in figure 6 and it is noticed that the refractive index has a maximum value of 2.15 at 355 nm for the pure isonitrosoacetophenone and the refractive index of the mixed one is shown in figure 7. The refractive indices of the material are an important physical property that must be evaluated before using the material in specific applications, such as optical and optoelectronic applications. The refractive indices of the material changes with the variation of the wavelength of the incident light beam.

The energy band-gap of the materials is determined using the reflection spectra. According to the Taucc's relation, the absorption coefficient, for direct ban-gap material is given by Sharma equation [10];

$$(a\upsilon)^n = C(h\upsilon - E_g) \qquad (4)$$

where (E$_g$) is the energy gap, (C) is constant which has different values at different transitions, (hυ) is the photon energy and (n) is an index number which assumes the values of 1/2, 3/2, 2 and 3 depending on the nature of the electronic

transition responsible for the reflection [11]. The value of the energy gap has been calculated by extrapolating the straight thin portion of the curve to intercept the energy axis [12]. The calculated band-gap energy of the pure isonitrosoacetophenone and of the mixed with water of different concentrations are shown in figure 8.
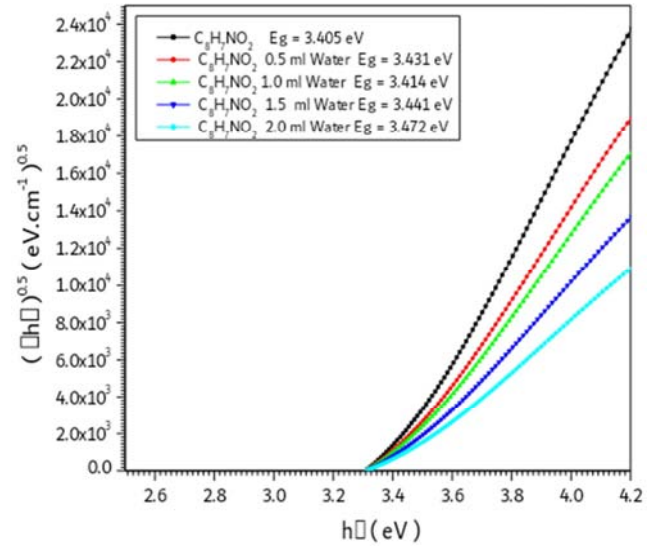
Figure 8. (ahυ)$^{0.5}$ against the energy of pure (C$_8$H$_7$NO$_2$) and that mixed with water for n=0.5.
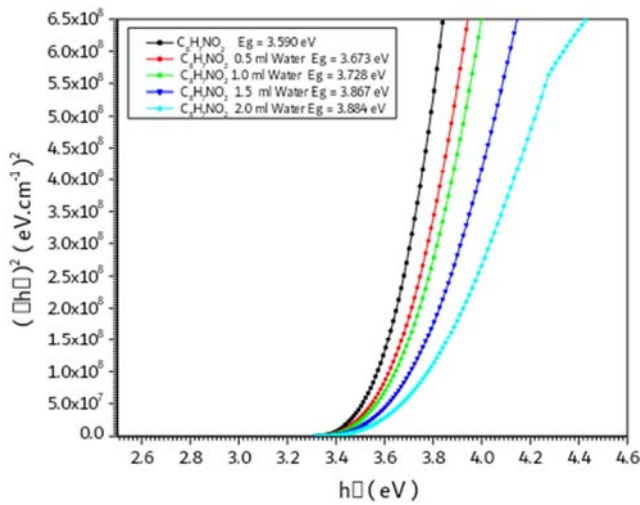
By means of plotting (αhυ)$^{0.5}$ versus photon energy hυ (direct allowed transition case) as shown in figure 8, the value of (Eg) was obtained by extrapolating of the resulting curve, and it was shown that its value is increased from (3.405) eV for pure C$_8$H$_7$NO$_2$ to (3.472) eV for (C$_8$H$_7$NO$_2$ with 2.0 ml water concentration). The increasing of (E$_g$) may be related to the change in the chemical bonding of the molecule (C$_8$H$_7$NO$_2$) when mixed with water.

Figure 9 shows the plot of (αhυ)$^{3/2}$ versus photon energy (hυ) of pure isonitrosoacetophenone and that mixed with different concentrations of distilled water.
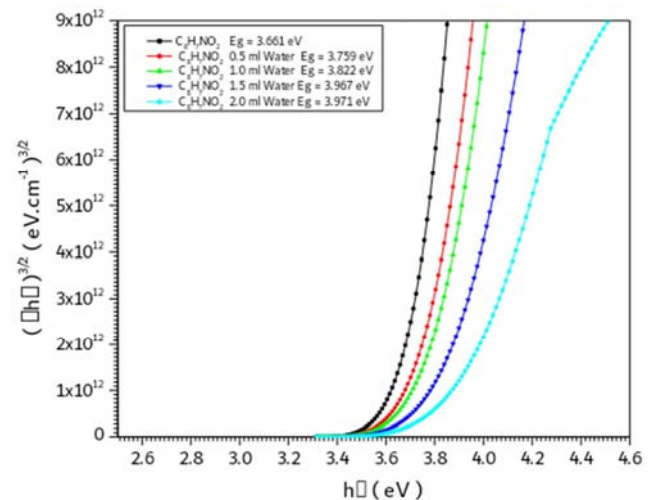
Figure 9. (ahυ)$^{3/2}$ against the energy of pure (C$_8$H$_7$NO$_2$) and that mixed with water for n=3/2.

As done in a previous approach (in case n=0.5), the $(\alpha h\upsilon)^{3/2}$ versus photon energy (hυ) was plotted and extrapolated, the value of (Eg) obtained for pure isonitrosoacetophenone was (3.661) eV and (3.971) eV for the mixed isonitrosoacetophenone with 2.0 ml water concentration. Therefore, the index number can also affect the band-gap calculation, for example when n=0.5 as shown in figure 8 and n=3/2 (forbidden direct transition) as shown in figure 9. Our aim in this part is to compare the band-gab of the pure and mixed isonitrosoacetophenone at the same index number at different water concentrations for the mixed one. Referring to figure 9, the increase in the concentration of water and/or the index number (n) results in the large band-gap. Figure 10 shows the obtained band gab for the pure and mixed isonitrosoacetophenone at index number n=2.

**Figure 10.** $(\alpha h\upsilon)^2$ against the energy of pure ($C_8H_7NO_2$) and that mixed with water for n=2.

Figure 10 shows the results of plotting $(\alpha h\upsilon)^2$ versus photon energy (hυ) for pure and mixed ($C_8H_7NO_2$) with different concentrations of water, and the extrapolation was used to obtain the values of the optical band-gap. As shown in figure 10, the optical band-gap for the pure isonitrosoacetophenone was 3.590 eV and mixed with 2.0 ml was 3.884 eV. Furthermore, the different concentrations of the water in the isonitrosoacetophenone compound were effected on its band-gap. Comparing the results obtained in figure 10 with those obtained in figures 8 and figure 9 it's clear that when n=0.5, the band gab values either for pure or mixed isonitrosoacetophenone are the lowest than its values when n=3/2 and 2. While comparing the band gab results either for pure or mixed isonitrosoacetophenone when n=3/2 and 2, it indicates that the band-gap values are large when n=3/2 than n=2, which corresponds to the indirect allowed transition.

For forbidden indirect transition cases when n=3, the plot of $(\alpha h\upsilon)^3$ versus photon energy (hυ) for pure and mixed isonitrosoacetophenone is shown in figure 11.

Figure 11 shows the values of the optical band gab of the pure and mixed isonitrosoacetophenone. The same ideas of

increasing the band gab as a result of water concentration also exist; therefore this result supported the previous discussion of the figures 8, 9, and 10. In addition, it is clear that the index number strongly affected the values of the band gab for either pure or mixed isonitrosoacetophenone compound.
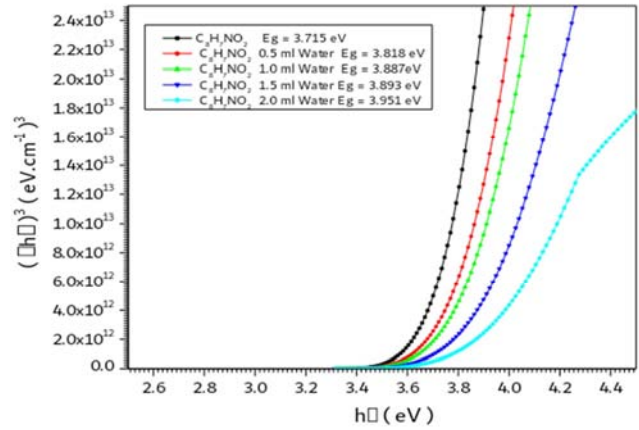
Figure 11. Spectrum of $(\alpha h\upsilon)^3$ against energy for five ($C_8H_7NO_2$) samples.

4. Conclusions

In conclusion, the optical properties of the isonitrosoacetophenone ($C_8H_7NO_2$) were studied using UV-Vis spectroscopy. It was shown that the value of the optical properties affected by the Isonitrosoacetophenone concentrations. The absorbance was shown to be decreased from 2.7×10^{-4} (a. u.) at 278 nm for pure isonitrosoacetophenone to 1×10^{-4} (a. u.) for mixed isonitrosoacetophenone with 2.0 ml at the same wavelength (278 nm). The transmission of the $C_8H_7NO_2$ was showed to shift towards the shorter wavelength as the concentration of water is increased, starting from ~346 nm for pure $C_8H_7NO_2$ and decreased to ~300 nm when the concentration of water was 2.0 ml. In addition, the results showed that more studies for $C_8H_7NO_2$ compound at the wavelength range from 220 to 300 nm are highly needed. The results of absorption coefficients of the five isonitrosoacetophenone are also supporting the above discussion, which is decreased as the concentration of water increased. Using the same concept that appeared from the results of the refractive indices of the pure and mixed $C_8H_7NO_2$, the refractive indices spectra (refractive indices vs. wavelengths) are shifted to the left. Nevertheless, the strange results from those obtained when the concentration of the water has increased the value of the refractive indices of the mixed $C_8H_7NO_2$ in the wavelengths range of (220-300) nm. Furthermore, it was shown that the value of band-gap (E_g) increased from (3.405) eV for pure $C_8H_7NO_2$ to (3.472) eV for mixed $C_8H_7NO_2$ with 2.0 ml water. Moreover, the results show that the band gap values of either pure or mixed $C_8H_7NO_2$ were increased as (n) increase, and it has higher values when n=3/2 than n=2 which corresponds to indirect allowed transition.

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