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Spectroscopic and Photonic Properties of Dexamethasone used in the Treatment of COVID-19 Patients

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ABSTRACT

Dexamethasone is a synthetic adrenal corticosteroid with potent anti-inflammatory properties. Dexamethasone (MK-125) is a position 9 fluorinated corticosteroid used to treat endocrine, rheumatic, collagen, dermatological, allergic, ophthalmic, gastrointestinal, respiratory, hematological, neoplastic, edematous, and other conditions. On June 16, 2020, a press release for the Randomized Evaluation of COVID-19 Treatment (RECOVERY) trial recommended the use of dexamethasone in COVID-19 patients with severe respiratory symptoms. Dexamethasone reduced deaths by approximately one-third in ventilated patients and one-fifth in patients requiring oxygen. Therefore, Dexamethasone is used in the treatment of COVID-19 patients in some countries. In this study, we researched the spectroscopic and photonic properties of Dexamethasone. We have extensively studied the absorption spectra at different concentrations and their response to light. This study shows the absorbance spectra of the Dexamethasone for various concentrations. On the other hand, we continue to work intensively on some herbal suggestions that can be considered equivalent to Dexamethasone.

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1. Introduction

Asthma, a complex and common chronic disease, has serious adverse effects such as bronchial hypersensitivity, intermittent airflow obstruction, and airway inflammation. This is due to allergic reactions. Decongestants, antihistamines, and corticosteroids are the three main drugs that can be used for this antiallergic effect and anti-inflammatory [1,2]. One type of corticosteroid is Dexamethasone. Dexamethasone plays an important role in the treatment of asthma, severe allergies and various skin diseases, especially by preventing the release of substances that cause inflammation in the body. The effects of dexamethasone are often seen within one day and persist for about three days [3,4]. Dexamethasone tablets are available and marketed under different brand names such as Decmax, Decdan, Daksone, Intradex, Dexasone, Demisone, and Dexona. In December 2019, there was an outbreak of a novel pneumonia-like illness in Wuhan, China. Clinical features included dry cough, fever and shortness of breath with lower respiratory tract involvement in patients confirmed to be infected with the novel coronavirus (SARS-CoV-2). The virus quickly spread around the world. It caused widespread panic, fear and death. According to a WHO report published on 7 September 2020, the virus then spread rapidly to more than 200 countries around the world, resulting in 27 million confirmed cases and 883,000 deaths worldwide. The COVID-19 pandemic is considered to be the most severe global pandemic for public health since the influenza pandemic of 1918 [5-7]. Three months after the outbreak of the coronavirus disease 2019 (COVID-19)1, caused by the severe acute respiratory syndrome coronavirus 2 (SARS-CoV-2), the World Health Organization declared it a pandemic. Estimates suggested that up to 12% of patients hospitalized with COVID-19 required invasive mechanical ventilation, with the majority developing acute respiratory distress syndrome (ARDS). A meta-analysis identified an association between corticosteroids and higher mortality in influenza patients. The findings of a randomized clinical trial involving COVID-19 patients showed that the use of dexamethasone reduced mortality in hospitalized patients requiring supplemental oxygen or mechanical ventilation. A randomized clinical trial of Dexamethasone (CoDEX) for COVID-19 was conducted to evaluate the efficacy of intravenous dexamethasone in patients with moderate to severe ARDS due to COVID-19. The hypothesis was that dexamethasone would increase the number of days alive and independent of mechanical ventilation during the first 28 days [8].

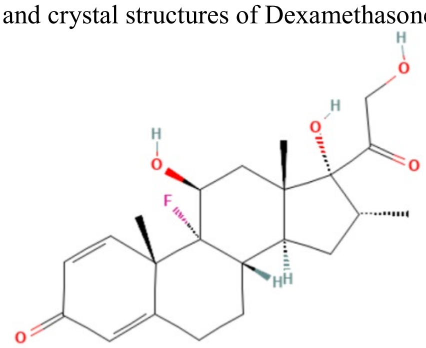
In this study, we investigated various spectroscopic and optoelectronic properties of dexamethasone and discussed its role in similar diseases, especially COVID-19, and its similarities and differences with thyme.

2. Experimental

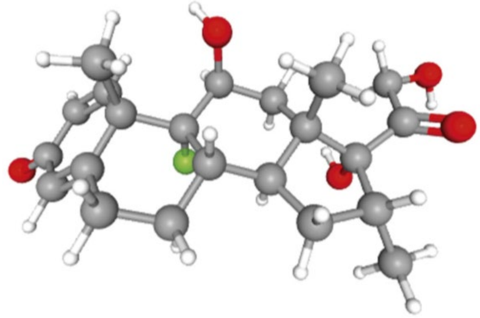
No analytical purity or purification was applied to the reagents and solvents used for dexamethasone measurements. All reagents were commercial purchases from Merck and Sigma-Aldrich, respectively. Optical measurements were carried out with the aid of a Shimadzu UV-1800 spectrophotometer in a range of solvents and at different molarities. Electronic spectra were measured using a Shimadzu model UV-1800 spectrophotometer in ethanol at 25°C in 1cm Quartz cells.

2.1. The Dexamethasone solutions and optical data

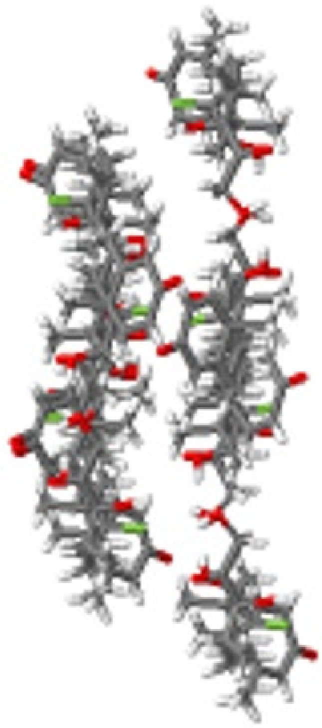
UV measurements of the drug dexamethasone for different molarities were performed using a Shimadzu model UV-1800 spectrophotometer with a cylindrical cuvette (Hellma QS-100). The wavelength was 190-1100 nm at room temperature. Samples of the drug dexamethasone were homogeneously dissolved in 12 mL of water, weighed using an analytical balance (AND-GR-200 series). In addition, the same volume of H_2O solvent (12 mL) was used to prepare solutions of the drug dexamethasone with different molarity, 7.12, 5.60, 3.88 and 1.36 mM. Figure 1 shows the 2-dimensional (2D), 3-dimensional (3D) chemical and crystal structures of Dexamethasone.



a)



b)



c)

Fig. 1. a) 2D [9], **b)** 3D [10] and **c)** crystal [11] structures of Dexamethasone.

2.2. Spectroscopic Properties

Fig. 2 shows the absorbance spectra of Dexamethasone for different concentrations. As seen in Fig. 2, the absorbance curves show dominant peaks in the UV-C region (in the wavelength range of about 200-280 nm). The maximum peak value is observed at about 241 nm. Minimum absorbance is observed in the UV-B and UV-A regions. As can be seen from the absorbance curves, the absorbance values increase as the concentration increases, as expected.

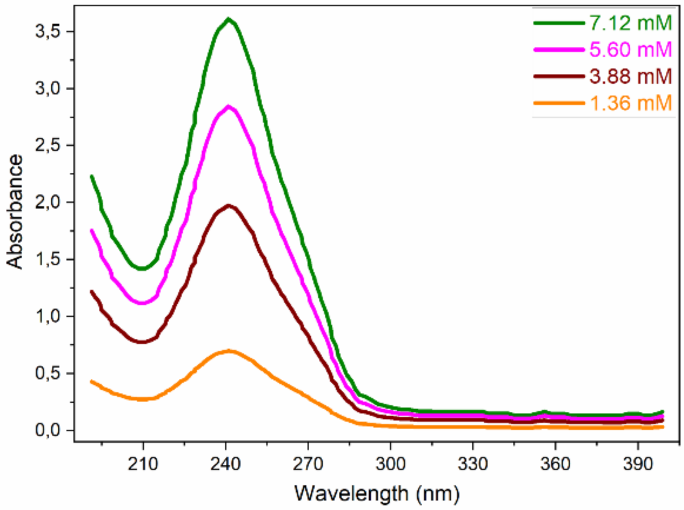


Fig. 2. Absorbance spectra of Dexamethasone for different concentrations.

On the other hand, Fig. 3 shows the UV-VIS spectra of unprocessed oregano essential oil (EO) and carvacrol given in a study in the literature [12]. As seen in Fig. 2 and 3, at the wavelengths where the maximum absorbance peak value of Dexamethasone is observed (around 240 nm), the minimum absorbance bottom values of unprocessed oregano essential oil (EO) and carvacrol are observed. In other words, there is an inverse relationship between medicinal drug (absorbance the most) and herbal medicine (absorbance the least). This gives very important and interesting results. For example, we attach importance to the conclusion that oregano and carvacrol can be used in the form of herbal medicine as an alternative to the medically used Dexamethasone.

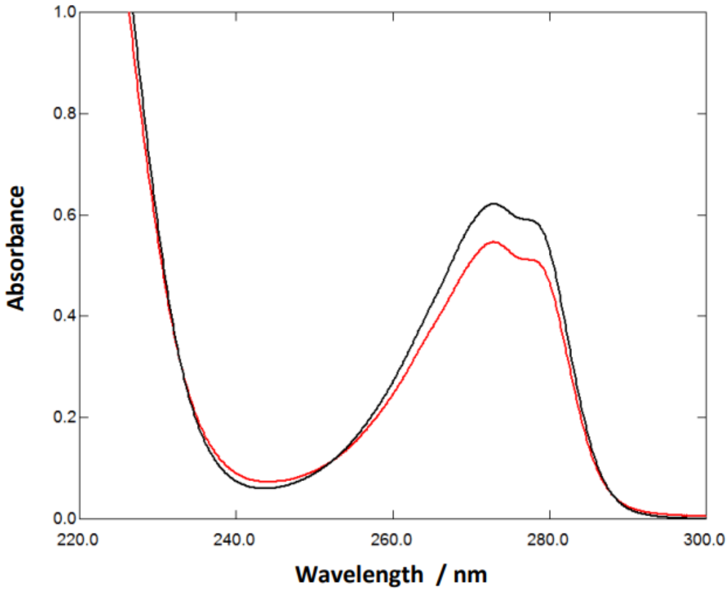


Fig. 3. UV-VIS spectra of unprocessed oregano EO (black line) and carvacrol (red line) [12].

The transmittance spectra of Dexamethasone for different concentrations are as seen in Fig. 4. In the UV-C and UV-B regions, the transmittance values increase sharply. Increasing the concentration causes a decrease in transmittance values.

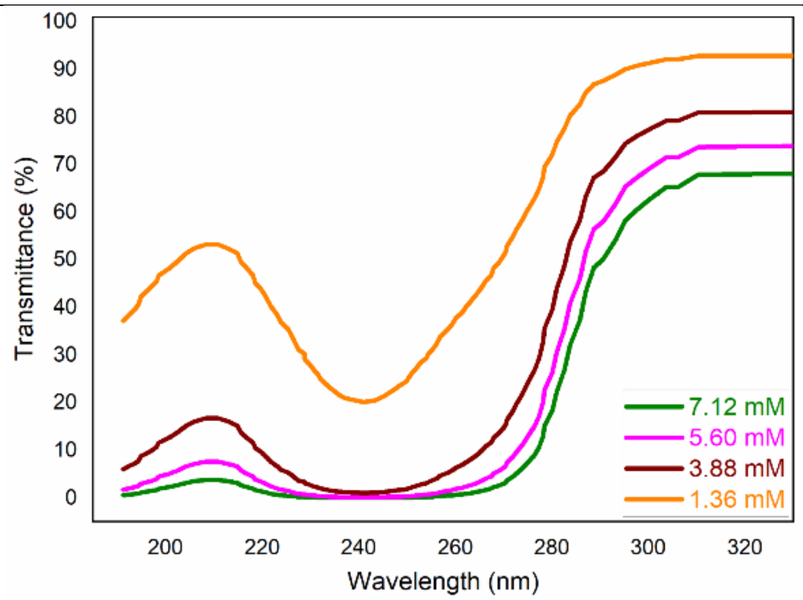


Fig. 4. Transmittance spectra of Dexamethasone for different concentrations.

2.3. Optical Band Gaps

The optical band gap (E_g) of optical transitions can be evaluated from the absorption spectrum using the Tauc relation [13,14],

$$(\alpha h\upsilon) = A(h\nu - E_g)^m \tag{1}$$

where A is a constant, hν is the photon energy, E_g is the optical band gap of the material and m is the parameter measuring type of band gaps. To determine the optical band gap of the Dexamethasone for different concentrations, the $(\alpha h\nu)^2$ plots vs. the photon energy (E) of the Dexamethasone are shown in Fig. 5. As seen in Fig. 5, there are linear regions for the direct optical band gap (E_{gd}) values of the Dexamethasone for different concentrations. By extrapolating the linear plot to $(\alpha h\nu)^2=0$, the E_{gd} values of the Dexamethasone for different concentrations were found.

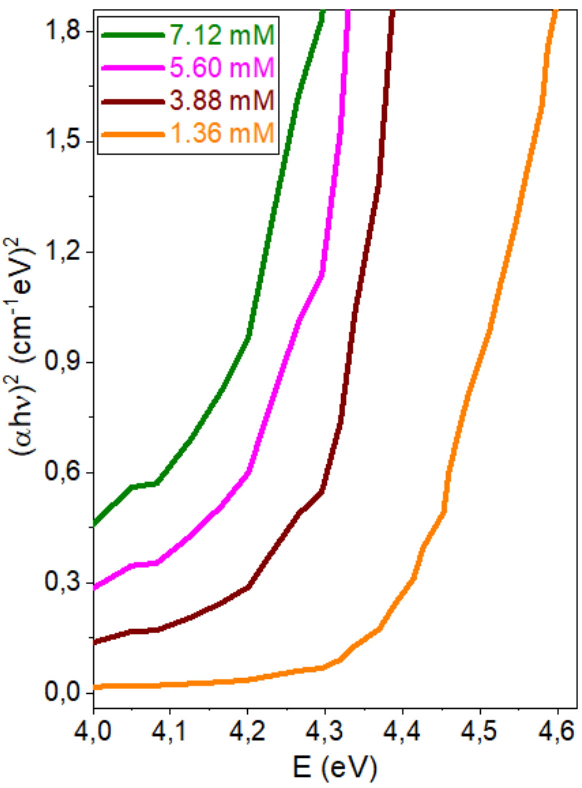


Fig. 5. The (αhν)2 curves vs. photon energy (E) of the Dexamethasone for different concentrations.

The E_{gd} values are given in Table 1. As can be seen in Table 1, the E_{gd} value (4.08 eV) of dexamethasone for 7.12 mM is the lowest. The E_{gd} value (4.38 eV) of Dexamethasone for 1.36 mM is the highest. The results obtained show that the lowest direct allowed band gap of the dexamethasone can be obtained with water as the solvent and that the E_{gd} value decreases with the increase of the molarity.

Table 1. Direct optical band gap (E_{gd}) of the Dexamethasone for different concentrations.

Solvents	**Molarity (mM)**	**E_{gd} (eV)**
H_2O	1.36	4.38
H_2O	3.88	4.27
H_2O	5.60	4.24
H_2O	7.12	4.08

2.4. Refractive Indices

The refractive index is one of the most important parameters for optical applications. Therefore, the determination of the optical constants of the drug under investigation, dexamethasone, is of vital importance for the solution of today's most important problems [15-17]. On the other hand, the refractive index can be also calculated by [18].

$$n = \left\{ \left[\frac{4R}{(R-1)^2} - k^2 \right]^{1/2} - \frac{R+1}{R-1} \right\} \quad (2)$$

The n values of the Dexamethasone for different concentrations were calculated from Eq. (2). Fig. 6 shows the n curves vs. angular frequency (ω) of the Dexamethasone for different concentrations. The Dexamethasone exhibits both the normal and abnormal dispersion property as seen in Fig. 6.

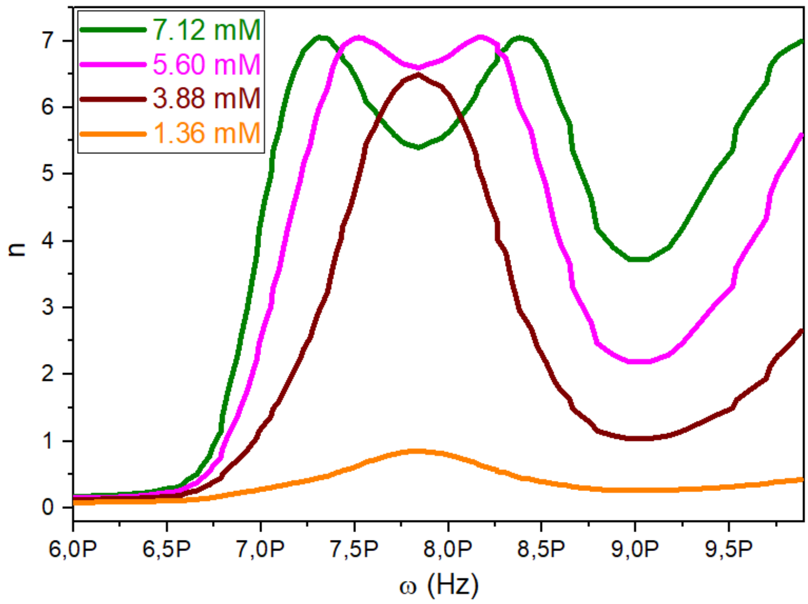


Fig. 6. The refractive indices of the Dexamethasone for different concentrations.

3. Conclusions

The spectroscopic properties of Dexamethasone were investigated experimentally. Dexamethasone can be used in optoelectronic applications that require non-semiconductor materials, especially insulating materials. Dexamethasone has band gaps and absorption band shores greater than 4. Dexamethasone can be used in photonic applications that require high reflectance, especially at low wavelengths. An herbal medicine with a minimum wavelength in the same range as the maximum wavelength of dexamethasone was investigated. It is recommended to compare thyme and Dexamethasone in future studies. The literature spectroscopic properties of Thyme/Oregano were also investigated and its comprehensive comparison was discussed. Thyme especially showed a reverse absorption feature with Dexamethasone, and its maximum and minimum relationship at the same wavelengths gives an important idea for medicinal and herbal medicines. Revealing the spectroscopic and photonic properties of dexamethasone makes a significant contribution to the literature, especially to the field of medicine and photonic technology.

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