Optical Characteristics of Vitamin D₃ Soft Gel

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Abstract
In this work, the linear properties of Vitamin D₃-5000IU soft gel were investigated by measuring its absorption and fluorescence spectra. It was observed that there was a shift towards longer wavelength within limits (75 nm), with quantitative efficiency equal to (33.58%). The values of absorbance were used to calculate the extinction coefficient, optical refractive index, optical conductivity and optical dielectric constant values.

The non-linear properties of Vitamin D₃-5000IU soft gel was also studied using the Z-Scan technique by using Neodymium-doped Yttrium Garnet (Nd: YAG) continuous laser (CW) emitting in (532 nm) wavelength, by utilize open aperture to measure nonlinear absorption coefficient and close aperture (diameter 1.5mm) to measure nonlinear refractive index. The sample behaves as two-photon absorption, and the nonlinear refractive index was positive.

1. Introduction
In the last years, there has been an imposing amount of academic survey and industrial research in the field of understanding the properties of "organic materials" due to the impressive growth in the number of proposed electronic devices, in addition to the increased interest in health care based on organic compounds. Nonlinear optics can be defined as a study of interaction between light intensity and mediums. Materials generally respond linearly to the amplitude of an electrical field. Presence of laser (high power) leads to rapid changes in the material properties and the occurrence of nonlinear effects [1]. The first one who introduced the Z-scan technique was Sheik Bahaet.al, which is based on the essentials of distorted of the beam, in addition to supply easy measurements with high sensitivity [2], and yields each of sign and magnitude of the nonlinearity, in addition to the value of the nonlinear refractive index by using minimum of analysis [3]. Where parameters of NLA and NLR are relying on the intensity of electric field for the laser light [4]. Pure Vitamin D₃ (Cholecalciferol), whose chemical structure is shown in Fig.1 [5], is absorbed at a maximum wavelength of (373 nm) and maximum fluorescence is at (475nm) [6, 7].

**Figure 1:** Chemical structure of Cholecalciferol [5].
The amount of vitamin D 5000 IU as (D₃ Cholecalciferol) per one soft gel equal to 1,250%, it also contains other ingredients such as "Soybean Oil", "Gelatin Vegetable" "Glycerin", "Corn Oil" and this component cause shifted and broad band to the peak of absorbance and fluorescence, which indicate that intermolecular interactions has occur between Vitamin D₃ and the other components [8].

Since Cholecalciferol is an organic substance that acts as a non-linear substance, as it has a displacement towards the longer wavelength (red shift) in some excited wavelengths, as it has been demonstrated in this research, therefore the non-linear properties and its potential use in optical applications were investigated and studied. So, the aim of this research is to study the optical properties (linear and non-linear) of Cholecalciferol which include absorption and fluorescence spectrum, quantum efficiency and FWHM, in addition to "nonlinear refractive index" and the "nonlinear absorption coefficient", and other parameters.

2. Experimental work

Vitamin D₃- 5000IU (Cholecalciferol), "Nature's Bounty Inc., USA, of the molecular formula (C₂₇H₄₄O), and molar mass of (384.64g/mole) were purchased from pharmacy of Baghdad, Iraq. The refractive index of vitamin D₃ gel was measured with a refractometer (Bellingham and Stanley Ltd, Tunbridgewells, ABBE60, England) and it was equal to (1.47523) at (20°C). Optical measurements were done in the range of wavelength between (200-800 nm) with Agilent Technologies Cary Eclipse Fluorescence Spectrophotometer (Malaysia). MATLAB 8 program was used to extract the values of the area under the absorption and fluorescence spectra in addition to the molar absorption coefficient. Therefore, the amount of energy absorbed by the dye molecules can be determined.

3. Results and discussion

Table 1 and 2 shows the most important spectral properties of the substance. Fig. 2 shows that the peak wavelength of the D₃ absorption and fluorescence spectra are at (364 nm) and (439.276 nm) respectively. The refractive index of vitamin D₃ gel was (1.47523) at (20°C). The obtained values of the absorbance were used by entering the information in a computer program (MATLAB 8) to calculate the values of the area under the curve of the absorption spectrum and fluorescence spectrum in order to get the value of quantum efficiency (qfm) by applying the Eq. (1):

\[
q_{fm} = \frac{\text{Number of Quanta Emitted}}{\text{Number of Quanta Absorbed}}
\]  

\[ (1) \]

| Maximum peak wavelength of absorption (ABS max.) (nm) | Absorption Intensity | Full width at half maximum of absorption spectrum (FWHM) (nm) | Maximum peak wavelength of fluorescence (F max.) (nm) | Fluorescence Intensity | Full width at half maximum of fluorescence spectrum (FWHM) (nm) | Stock shift (nm) |
|------------------------------------------------------|----------------------|-------------------------------------------------------------|------------------------------------------------------|-----------------------|-------------------------------------------------------------|----------------|
| 364                                                  | 537.314              | 127.1178                                                    | 439.276                                              | 161.597               | 109.6251                                                    | 75.276         |

Table 1: The (absorption, fluorescence) wavelength at relative maximum intensity; full width at half maximum (FWHM) and stock shift of Vitamin D₃ gel.
Table 2: Quantum efficiency; non-radiative and fluorescence life time of Vitamin D₃ gel.

| Quantum efficiency % | Radiative emission probability (Kₘ(fm)) | Non-radiative life time tₘ (nsec) | fluorescence life time tᵣ (nsec) |
|----------------------|----------------------------------------|----------------------------------|---------------------------------|
| 33.58302             | 2.0334                                 | 0.4917                           | 0.1651                          |

Also, the information we obtained enables us to calculate the value of radiative emission probability (Kₘ(fm)) Eq. (2), and non-radiative life time (τₘ(fm)) Eq. (3), by Bowen-wokes equation [9]:

$$K_{fm} = \frac{1}{\tau_{fm}} = 2.88 \times 10^{-9} \times n^2 \times \int \varepsilon(\nu)d\nu$$  \hspace{1cm} (2)

where (n) refractive index, (ε) molar absorption coefficient, (ν) wave number. The fluorescence life time (τᵣ) was calculated from the following equation:

$$\tau_f = q_f \times \tau_{fm}$$  \hspace{1cm} (3)

where (qᵢ) represents quantum efficiency.

Origin (9.1) "data analysis and graphing software” was used to calculate the value of (FWHM) for the absorption and fluorescence curves and which were (127.1178nm) and (109.6251nm) respectively, because it is not pure and contain the above substances which effect on the curved width. Energy band gap values [10] can be extracted from the relation between photon energy and (αhν)², where their value was equal to (2.7 eV) as shown in Fig.3, Table 3.

Figure 2: Absorption and Fluorescence spectrum of Vitamin D₃ gel.

Figure 3: Energy gap assessment for Vitamin D₃ gel.
Table 3: Optical parameters of Vitamin D$_3$ gel.

| Sample          | Energy band gap (eV) | Extinction coefficient (k) (no unit) | Optical refractive index(n) (no unit) | Optical conductivity ($\sigma$) (Ω$^{-1}$cm$^{-1}$) | Real dielectric constant (no unit) ($\varepsilon_r$) | Imaginary dielectric constant (no unit) ($\varepsilon_i$) |
|-----------------|----------------------|-------------------------------------|--------------------------------------|-----------------------------------------------|-------------------------------------------------|-------------------------------------------------|
| Vitamin D$_3$ gel | 2.7                  | 0.003586                            | 2.003722                             | 619.868564                                    | 4.01489                                         | 0.014371                                        |

In addition, the absorption spectra data can be useful to extract "extinction coefficient" (k) Fig. 4, "optical conductivity" ($\sigma$) Fig. 5, "optical refractive index" (n) Fig. 6, and {real($\varepsilon_r$) and imaginary ($\varepsilon_i$)}" optical dielectric constant"values Fig. 7 and 8, which are shown in Table 3, using the following equations [11-16]:

\[
K = \frac{\alpha \lambda}{4\pi} \tag{4}
\]

\[
n = \frac{1 + R}{1 - R} \left( \frac{4R}{(1 - R)^2} - K^2 \right) \tag{5}
\]

where $\alpha$ is the absorption coefficient and equal to {($\alpha = 2.303*A/I$), A is the absorbance, I is the thickness, $\lambda$ is the "incident photon" wavelength and R is the reflection.

\[
\sigma = \frac{\alpha n}{4} \tag{6}
\]

\[
\varepsilon_r = n^2 - K^2 \tag{7}
\]

\[
\varepsilon_i = 2nK \tag{8}
\]

The extinction coefficient depends on absorbance according to Eq. (4), so the behavior of Vitamin D$_3$ gel was comparable to the absorption spectrum. The real dielectric constant depends on the value of ($n^2$) and ($K^2$) hence the similarities of the curve of refractive index.

The nonlinear absorption coefficient ($\beta$) was calculated using experiments of open Z-scan aperture and applying the following Equations [17-19]:

\[
T(Z) = \sum_{m=0}^{\infty} \left( \frac{-q_o}{m+1} \right)^m \tag{9}
\]

\[
q_o(Z) = \frac{I_0 L_{\text{eff}} \beta}{1 + \left( Z/Z_0 \right)^2} \tag{10}
\]

where $T(Z)$ is the normalized transmittance of the sample when at position Z, $I_0$ is the laser beam Intensity at focus z = 0, Z is the position of the sample with respect to the focal position, $Z_0$ is the Rayleigh range ($= n\pi(w_0)^2/\lambda$), and $L_{\text{eff}}$ is the effective thickness of sample.
While the nonlinear refractive index \( n_2 \) was calculated by the experiments of close Z-scan aperture with pinhole diameter (1.5mm) and applying the following equations:

\[
n_2 = \frac{\Delta \Phi_o}{I_0 L_{off} K} \quad (11)
\]

\[
\Delta T_{P-V} = 0.406 |\Delta \Phi_o| \quad (12)
\]
\[ L_{\text{eff}} = \frac{(1 - e^{-\alpha z})}{\alpha} \]  

(13)

where \( L \) is the sample thickness, \( \Delta \Phi_0 \) is the nonlinear phase shift, \( k \) is the wave number, and \( \Delta T_{p-v} \) is the difference value between the normalized (peak and valley). Experiments of open and close Z-scan aperture were used in order to calculate the nonlinear absorption coefficient (\( \beta \)), and the nonlinear refractive index of vitamin D\(_3\). Fig. 9 shows transmittance of laser beam after passing through vitamin D\(_3\) sample, the "nonlinear absorption coefficient" of the sample exhibits the behavior of two-photon absorption and this is the resultant of changing the intensity of the laser moving through the beam waist on the sample. Fig. 10 shows the closed aperture curve which indicates that the value of the nonlinear refractive index is positive which means self-focusing, and Table 4 shows the nonlinear properties of Vitamin D\(_3\).

![Open aperture Z-scan measurements of Vitamin D\(_3\)-5000IU soft gel.](image1)

![Close aperture Z-scan measurements of Vitamin D\(_3\)-5000IU soft gel.](image2)

**Table 4: Nonlinear properties of Vitamin D\(_3\)-5000IU soft gel.**

| ABS. Intensity at 532nm | \( \alpha \) (cm\(^{-1}\)) | \( L_{\text{eff}} \) (cm) | \( T(z) \) | \( \beta \) (cm/W) | \( \Delta T_{p-v} \) | \( \Delta \Phi_0 \) x10\(^6\) | \( n_2 \) x10\(^{-8}\) (cm\(^2\)/W) |
|-------------------------|-----------------|-----------------|--------|-----------|--------|-----------------|----------------|
| 169.524                 | 7808.2754       | 0.000128        | 0.006437 | 1546.4804 | 0.004684 | 2.5034          | 1.16706        |

**4. Conclusions**

The optical properties of the Vitamin D\(_3\) gel were investigated in the UV region. The calculated results showed that there was a shifting towards long wavelength and the (absorption, fluorescence) curves were broad due to the impurities which are already exists in the capsule. Quantum efficiency gain was (33.5%). The value of the energy gap was equal to \( (2.7\text{e.V}) \). The nonlinear absorption coefficient for Vitamin D\(_3\) behaved as two-photon absorption, and the nonlinear refractive index was positive.

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**Conflict of interest**

Authors declare that they have no conflict of interest.
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الخواص البصرية لفيتامين D$_3$ (هلام مرن)

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الخلاصة

في هذا العمل تم دراسة الخواص الخطية للهلام المرن لفيتامين D$_3$-5000IU عن طريق قياس أطيفات الامتصاص والفلورة، وقد وُجد أن هناك تحولاً نحو الطول الموجي الأطول ضمن حدود (75 نانومتر)، بكفاءة 33.58%. تم استخدام قيم الامتصاصية لحساب معامل الانكسار، معامل الأمتصاص البصري، الموصلية الضوئية وقيم ثابت العزل الكهربائي. Z-Scan أيضاً باستخدام تقنية D$_3$-5000IU تم دراسة الخواص غير الخطية للهلام المرن لفيتامين (Nd: YAG) باستخدام الليزر مخدر بعقيق الإتريوم (YAG) بالطفل المتوسط البصري بطول الموجي (532 نانومتر) باستخدام الفتحة المفتوحة. قيم معامل الامتصاص اللاخطي الفتحة المغلقة (قطر 1.5 مم) لقياس معامل الانكسار اللاخطي. تتصرف العينة كامتصاص فوتوني، وكان معامل الانكسار اللاخطي موجبًا.