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Optical Characteristics of Vitamin D_3 Soft Gel

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Abstract

In this work, the linear properties of Vitamin D_3-5000IU 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 D_3-5000IU 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.

Article Info.

Keywords:
Vitamin D, quantum efficiency, Z-scan.

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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 Sheikh Bahaeet.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 D_3 (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].

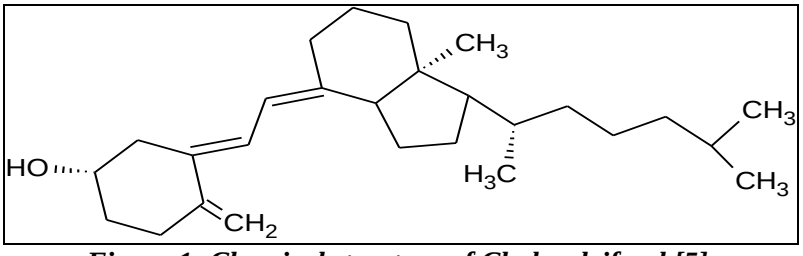

Figure 1: Chemical structure of Cholecalciferol [5].

The amount of vitamin D 5000 IU as (D_3 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 D_3 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 D_3- 5000_{IU} (Cholecalciferol), "Nature's Bounty Inc., USA, of the molecular formula ($C_{27}H_{44}O$), and molar mass of (384.64g/mole) were purchased from pharmacy of Baghdad, Iraq**.** The refractive index of vitamin D_3 gel was measured with a refractometer (Bellingham and Stanley Ltd, Tunbridgewells, ABBE60, England) and it was equal to (1.47523) at ($20C^{o}$). 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 D_3 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 ^{O}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 (q_{fm}) by applying the Eq. (1):

$$q_{fm} = \frac{Number\,of\ Quanta\ Emitted}{Number\,of\ Quanta\ Absorbed} \qquad \textbf{(1)}$$

Table 1: The (absorption, fluorescence) wavelength at relative maximum intensity;full width at half maximum (FWHM) and stock shift of Vitamin D_3 gel.

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 2: Quantum efficiency; non-radiative and fluorescence life time of Vitamin D_3 gel.

Quantum efficiency %	Radiative emission probability (K_{fm})	Non-radiative life time t_{fm} (nsec)	fluorescence life time t_f (nsec)
33.58302	2.0334	0.4917	0.1651

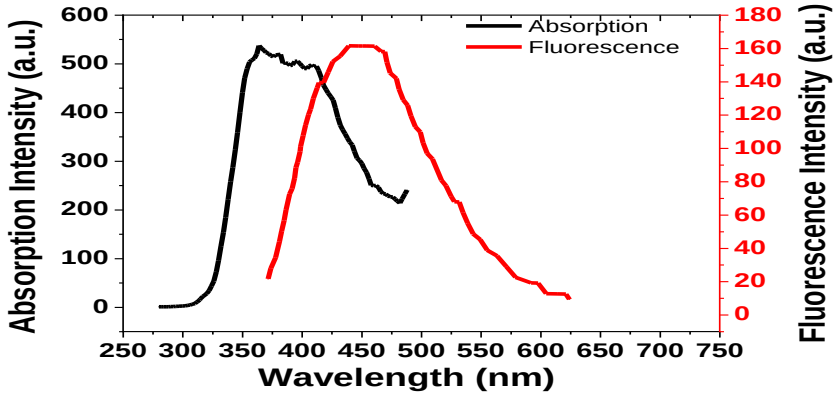

Figure 2: Absorption and Fluorescence spectrum of Vitamin D_3 gel.

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

$$K_{fm} = \frac{1}{\tau_{fm}} = 2.88\times10^{-9} \times n^2 \times (\bar{\upsilon}^2) \int \varepsilon(\bar{\upsilon}) d\bar{\upsilon} \qquad (2)$$

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

$$\tau_f = q_f \times \tau_{fm} \qquad (3)$$

where (q_f) 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 $(\alpha h\upsilon)^2$, where their value was equal to (2.7 eV) as shown in Fig.3, Table 3.

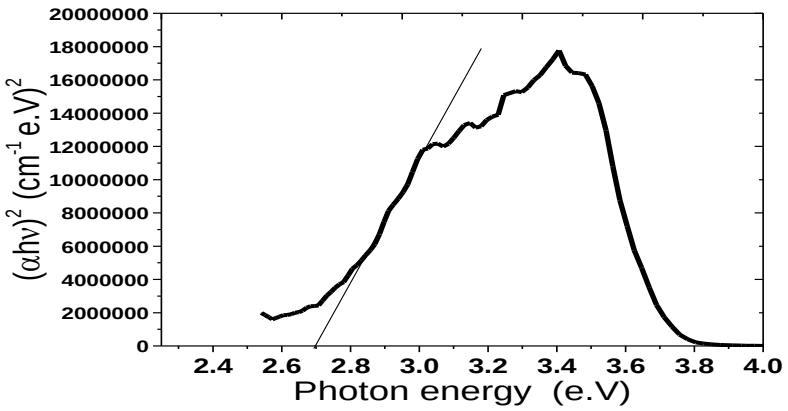

Figure 3: Energy gap assessment for Vitamin D_3 gel.

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 (σ) ($\Omega^{-1}.cm^{-1}$)	Real dielectric constant (no unit) (ε_r)	Imaginary dielectric constant (no unit) (ε_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" (σ) Fig.5, "optical refractive index" (n) Fig.6, and {real(ε_r) and imaginary (ε_i)}" optical dielectric constant"valuesFig.7 and 8, which are shown in Table 3, using the following equations [11-16]:

$$K = \frac{\alpha\lambda}{4\pi} \quad (4)$$

$$n = \frac{1+R}{1-R}\sqrt{\frac{4R}{(1-R)^2} - K^2} \quad (5)$$

where α is the absorption coefficient and equal to {(α=2.303*A/I), A is the absorbance, I is the thickness, λ is the "incident photon" wavelength and Ri s the reflection**.**

$$\sigma = \frac{\alpha n}{4} \quad (6)$$

$$\varepsilon_r = n^2 - K^2 \quad (7)$$

$$\varepsilon_i = 2nK \quad (8)$$

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 (β) was calculated using experiments of open Z-scan aperture and applying the following Equations [17-19]:

$$T(Z) = \sum_{m=0}^{\infty} \frac{(-q_o)^m}{(m+1)^{\frac{3}{2}}} \quad (9)$$

$$q_o(Z) = \frac{I_O L_{eff}\beta}{1+\frac{Z^2}{Z_O^2}} \quad (10)$$

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_{eff} is the effective thickness of sample.

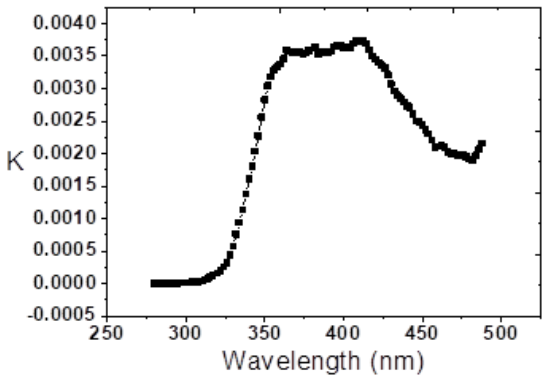

Figure 4: Relation between K and wavelength for Vitamin D_3 gel.

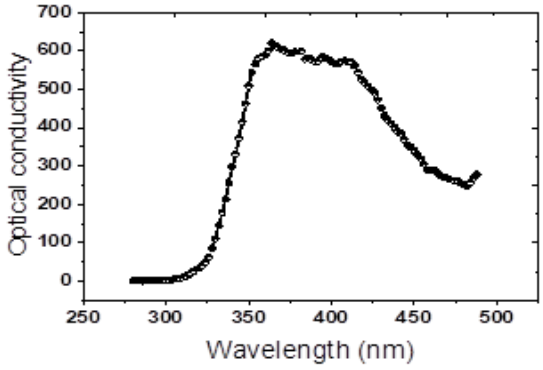

Figure 5: Relation between optical conductivity and wavelength for Vitamin D_3 gel.

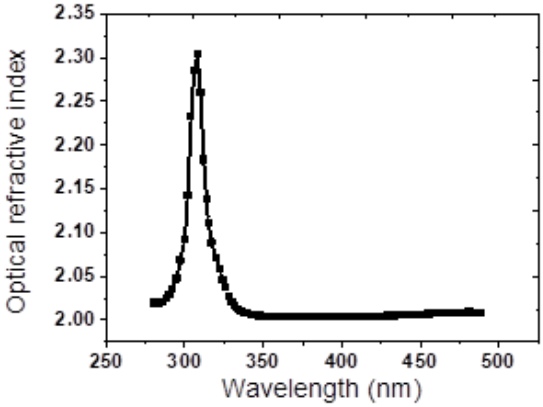

Figure 6: Relation between wavelength and optical refractive index.

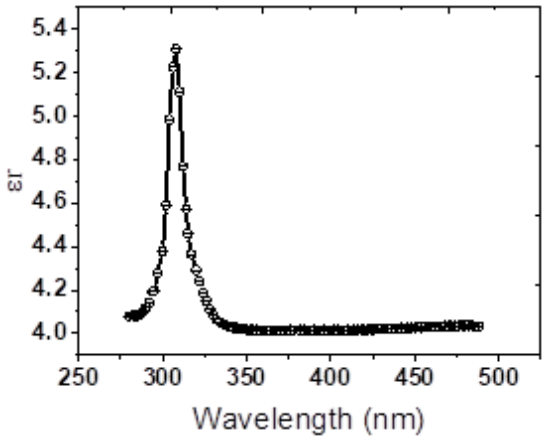

Figure7: Relationship between realdielectric constant and wavelength for Vitamin D_3 gel.

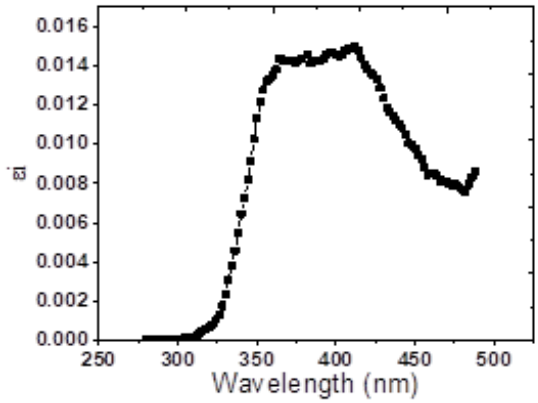

Figure 8: Relationship between imaginary dielectric constant and wavelength for Vitamin D_3 gel.

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:

$$n_2 = \frac{\Delta\Phi_o}{I_0 L_{eff} K} \qquad (11)$$

$$\Delta T_{P-V} = 0.406|\Delta\Phi_O| \qquad (12)$$

$$L_{eff} = \frac{(1-e^{-\alpha L})}{\alpha} \quad (13)$$

where L is the sample thickness, $\Delta\Phi_o$ is the nonlinear phase shift, k is the wave number, and ΔTp-v is the difference value between the normalized (peak and valley. Experiments of open and close Z-scan aperture was used in order to calculate the nonlinear absorption coefficient (β), 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.

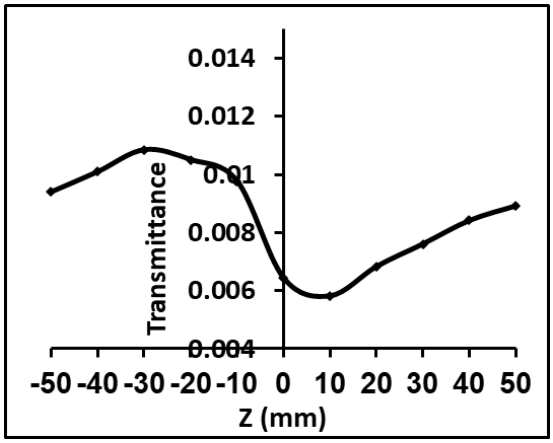

Figure 9: Open aperture Z-scan measurements of Vitamin D_3-5000IU soft gel.

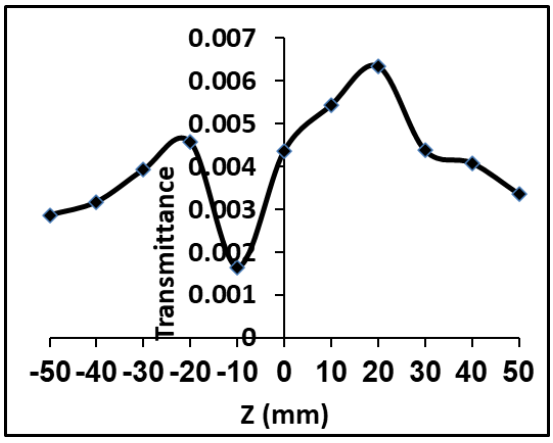

Figure 10: Close aperture Z-scan measurements of Vitamin D_3-5000IU soft gel.

Table 4: Nonlinear properties of Vitamin D_3-5000IU soft gel.

ABS. Intensity at 532nm	α (cm^{-1})	L_{eff} (cm)	T(z)	β (cm/W)	ΔT_{pv}	$\Delta\Phi_0$ $x10^{-6}$	$n_2 x10^{-8}$ (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 (2.7e.V). The nonlinear absorption coefficient for Vitamin D_3behavedas two-photon absorption, and the nonlinear refractive index was positive.

Acknowledgments

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Conflict of interest

Authors declare that they have no conflict of interest.

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الخواص البصريه 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 أطياف الامتصاص والفلورة، وقد لوحظ أن هناك تحولا نحو الطول الموجي الأطول ضمن حدود (75 نانومتر) ، بكفاءة كمية تساوي (33.58٪). تم استخدام قيم الامتصاصية لحساب معامل الاخماد، معامل الانكسارالبصري، الموصلية الضوئية وقيم ثابت العزل الكهربائي.

تمت دراسة الخواص غيرالخطية للهلام المرن لفيتامين D_3-5000IU أيضًا باستخدام تقنية Z-Scan باستخدام النيوديميوم المخدر بعقيق الإيتريوم (Nd: YAG) لليزر مستمرمنبعث بالطول الموجي (532نانومتر)، باستخدام الفتحة المفتوحة. لقياس معامل الامتصاص اللاخطي والفتحة المغلقة (قطر 1.5 مم) لقياس معامل الانكسار اللاخطي. تتصرف العينة كامتصاص فوتونين، وكان معامل الانكسار اللاخطي موجبًا.