STUDY OF ELECTRICAL ENERGY LEVELS OF THE LASER ACTIVE MEDIUM

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ABSTRACT

In this paper has been studied the electrical energy levels of molecules experimentally. The study was conducted using different concentrations solvents to see the effect of concentrations - (0.5 x 10^{-3}, 1x10^{-3}, 0.5x10^{-4}, 1x10^{-4},1x 10^{-5}) Ml to pop pop dye with chloroform- on the absorption and fluorescence spectra and linear optical properties (absorption coefficient, refractive index, life time and quantum yield of florescence level). Ranged wavelengths of the absorption spectra for pop pop solutions between (352-337)nm in chloroform. All these wavelengths within the transitions in molecular electrical orbits at type ($n\rightarrow\pi^*$).

The results were shifted absorption and emission (fluorescence) spectra peaks toward shorter wavelengths (blue shift), and increase the value of linear absorption coefficients and linear refractive index when increasing the concentration of the solution. It shows through the results that the life time of fluorescence increases and quantum yield decreases with increasing concentration of the solution.

Keywords: Electrical energy levels, Laser spectral ranges

INTRODUCTION

Action Laser extends the wavelength range from the near UV (336nm) through the near-infrared (1.8 micron). General classes of dyes and laser spectral ranges of the work. Emissions and increase the spectra of very wide range of organic dyes leads to a tunable laser output is usually over several tens of nanometers. Because of this property, it is used for dye lasers are widely used in spectroscopy wavelength selective.[1]

In 1993, (Mehdi Saleh) to study the spectral dye POPOP and C_{102} were thawing dye different solvents were prepared with different concentrations was observed for the removal of the absorption and fluorescence spectra.[2]

THEORETICAL PART

Is the total number of energy levels for any Molecule is very large as well as the energy must Divided into different energies by the equation:

$$\mathbf{E_{total} = E_T + E_N + E_R + E_V + E_E}$$

Where: $\mathbf{E_T}$:a transitional energy, $\mathbf{E_N}$:nuclear energy.

$\mathbf{E_E}$:Electronic energy . $\mathbf{E_R}$:Rotational energy. $\mathbf{E_V}$: vibratory energy.

Linear Optical Properties

For information about the internal structure of matter and the nature of its ties must know transmittance and absorbance and the reflectivity of the electromagnetic beam incidence on the material, for example, power packs and quality of transitions within the material

ISSN: 2223-9944, e ISSN: 2223-9553

identified studying the ultraviolet spectrum, but to see the area of the operation involving the use of materials applications must study the visible spectrum [3].

Absorbance(*A*)

The mathematical quantity linking density of particles (concentration) in the sample and the sample thickness (optical path length) is the absorbance (A) or optical density (Optical Density).

Absorption Coefficient (α_o)

Absorption coefficient is defined as the percentage decrease in the iceberg incident radiation energy per unit distance direction of wave propagation in the medium, and depends on the energy of the photon absorption coefficient (hυ) and on the properties of material [4].

Transmittance (T)

Can know the permeability of the center as "the percentage of the intensity of transmitted light (I) to the intensity of incident light (I_0) ", or as a "permeation of radiation energy from the medium to the incident radiation energy it " [5,6].

Refractive Index (n)

All light wave lengths at full speed it travels through a vacuum, a constant amount of this value and less than in any other medium, as they change in the material medium in different wavelengths. It defines the ratio between the speed of light in a vacuum to the speed at any particular center of a particular wavelength by a factor of refraction medium that wave [7].

Reflectance(R)

The reflection the light is known as bounce incident light on the surface separating two different Ogg in optical density, known as the reflective the energy of the reflected light.

Quantum Efficiency (Q_{FM})

Which represents the ratio between the numbers of photons emitted fluorescence to number pumping of photons absorbed by the dye molecule

$$q_{FM} = \frac{\text{Number of quanta emitted}}{\text{Number of quanta absorbed}} \quad \ldots\ldots\ldots(1)$$

Fluorescence

Sometimes irradiated system absorbed high amount of energy, which causes some of the electrons to much higher energy levels of the level of stability of the molecule, in this case the system can return to the level of stability directly launching photons have the same energy photons absorbed or can the electrons return to the case of stable stages of sequential launching photons of energy corresponding to the energy difference between the various stages of any less energy and the length of the longest wave of the absorbed originally and this is what is known fluorescence [8,9].

Fluorescence Lifetime(τ_F)

After absorbing particle of light emitted from an external source, they move to a vibrating electronic state levels irritated (S_n) and as a result of collisions with its neighboring molecules if Condensed Phase leading to the loss of part of its energy vibrational would drop to the lowest level for the case of unilateral irritated (S_1) and this level radiation transmitted to a

ISSN: 2223-9944, e ISSN: 2223-9553

vibrational levels of the ground state (S_0), this process occurs very quickly and very short times [10].

Experimental Part

2,2-p-pheny lenbis (5-pheny loxazole) Its scientific name Or P-Bis (5-pheny loxazole1) benzene. Molecular formula $C_{24}H_{16}N_2O_2$, Its molecular weight: Mol.Wt.364.4

Chemical composition:

Belong to this dye oxazole derivatives group and this group of episodes hybrid compounds (Hetrocyclic Compounds), which contains the rings on oxygen or nitrogen atom.[11,12]

Samples and methods of preparing the composition solution (dye + solvent) using the following equation:

$W=(Mw . C .V)/1000$ …….(2)

Where:

Mw: molecular weight of the dye

C: concentration of the solution required, V : solution size record

To prepare different concentrations of focus record using the following equation mitigation:

$C_1V_1=C_2V_2$……(3)

Where:
C_1 : focus of the first solution.
V_1 : size of the initial solution.
C_2 : concentration of second solution.
V_2 : second volume of the solution.

THE RESULTS

Samples were prepared from dyes to measure the concentrations and different solvents, Where properties were studied non-linear optical dye the popop different concentrations and different types of solvents as well as the spectrum of fluorescence dye laser.[13]

It was prepared five different concentrations(1×10^{-3}, 0.5×10^{-3} , 1×10^{-4}, 0.5×10^{-4}, 1×10^{-5}) M after dissolving dye the Popop in a solvent chloroform (Dichloromethane $CHCL_3$) . Where it was measured spectra of absorption and spectrum of fluorescence.

ISSN: 2223-9944, e ISSN: 2223-9553

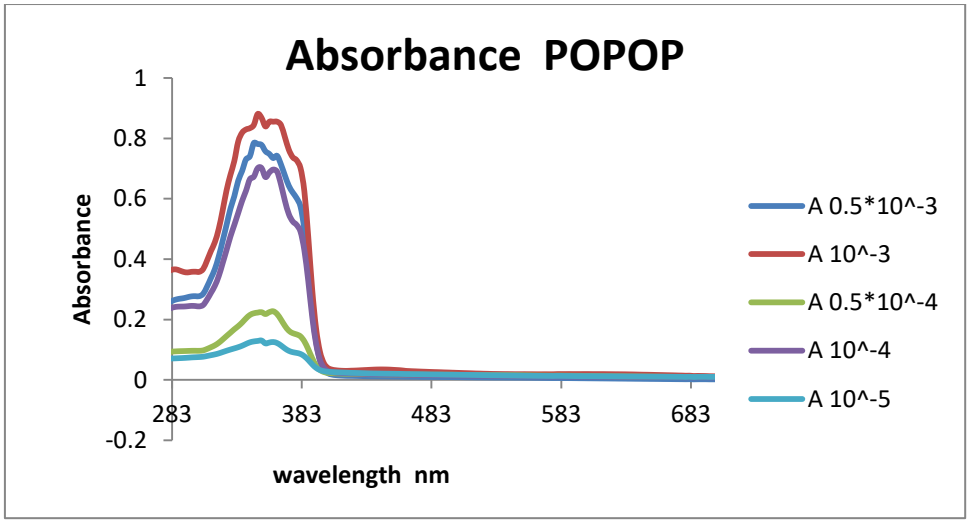

Figure 1. Absorption spectrum in the region (UV-VIS) for the solution popop dye dissolved in chloroform at different concentrations

Table 1. Absorbance in most wavelengths of popo dye dissolved in chloroform and different concentrations

C (M)	λ_{max} *(nm)*	*A*
$10^{-3}\times1$	352	0.8006
$10^{-3}\times0.5$	349	0.7650
$10^{-4}\times1$	346	0.6726
$10^{-4}\times0.5$	340	0.2037
$10^{-5}\times1$	337	0.1245

Note of the results and figure that decrease the concentration of the dye solution leads to the summit overtaken absorption spectra toward short wavelengths (blueshift).

One result of absorption spectra was obtained transmission spectra As shown in the figure (2).

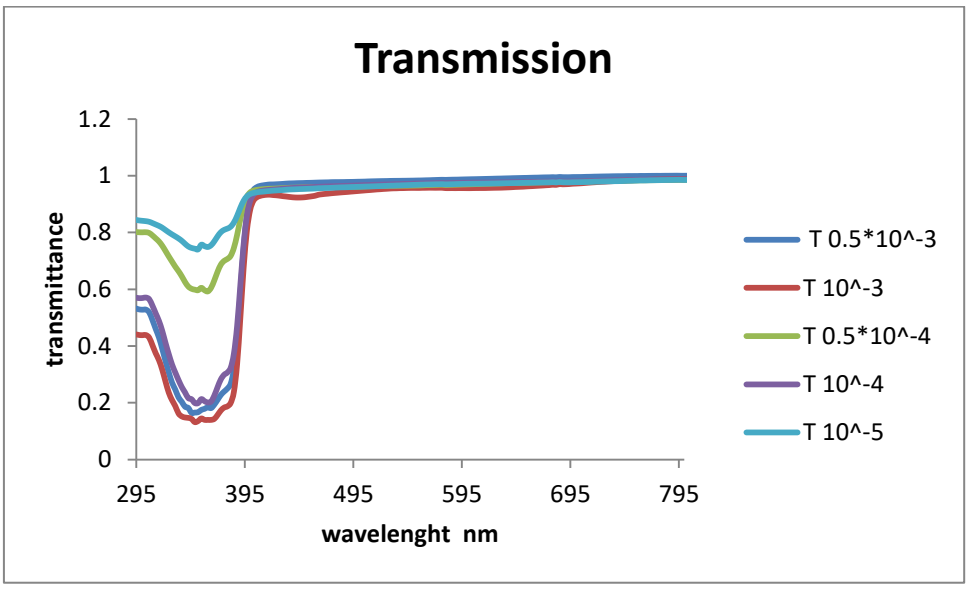

Figure 2. Spectrum transmittance in the region (UV-VIS) for the solution of the dye dissolved in chloroform popup at different concentrations

ISSN: 2223-9944, e ISSN: 2223-9553

Table 2. Transmittance in most wavelengths of popo dye dissolved in chloroform and different concentrations

C (M)	λ_{max} *(nm)*	*T*
$10^{-3}\times1$	343	0.1623
$10^{-3}\times0.5$	340	0.2163
$10^{-4}\times1$	340	0.2364
$10^{-4}\times0.5$	337	0.6457
$10^{-5}\times1$	334	0.779

After obtaining the results of transmittance were measured linear absorption coefficients (α_o) and linear refractive index (n_o) and Suppressions coefficient (K) models prepared after the introduction of three relationships (4) , (5) and (6) respectively in the software program, as shown in the table (3). [14,15]

$$K = \frac{\alpha_0 \lambda}{4\pi} \dots\dots\dots\dots\dots\dots\dots\dots (5)$$

$$n_o = \frac{1}{T} + [(\frac{1}{T^2} - 1)]^{1/2} \dots\dots\dots\dots (6)$$

Table 3. Linear absorption coefficient (α_o) and linear refractive index (n_o) and extinction coefficient (K)

C (M)	$)cm^{-1}$ $(\alpha_o$	$K*10^{-10}(m)$	n_o
$10^{-3}\times1$	2.263	6.338	1.5909
$10^{-3}\times0.5$	1.8539	5.416	1.5209
$10^{-4}\times1$	1.614	4.443	1.2074
$10^{-4}\times0.5$	0.4691	1.269	0.9518
$10^{-5}\times1$	0.2604	0.698	0.1437

It observed by the results that Change the concentration of the dye solution has a great effect on the nonlinear optical properties (refractive index and absorption coefficient of linear) for the absorption spectra and transmittance, where greater emphasis is increasing the refractive index and the absorption coefficient.

It was measured fluorescence spectra of samples prepared to dye solution (popop + chloroform) using a fluorescence spectrometer and the results of the measurements as shown in the figure 3.

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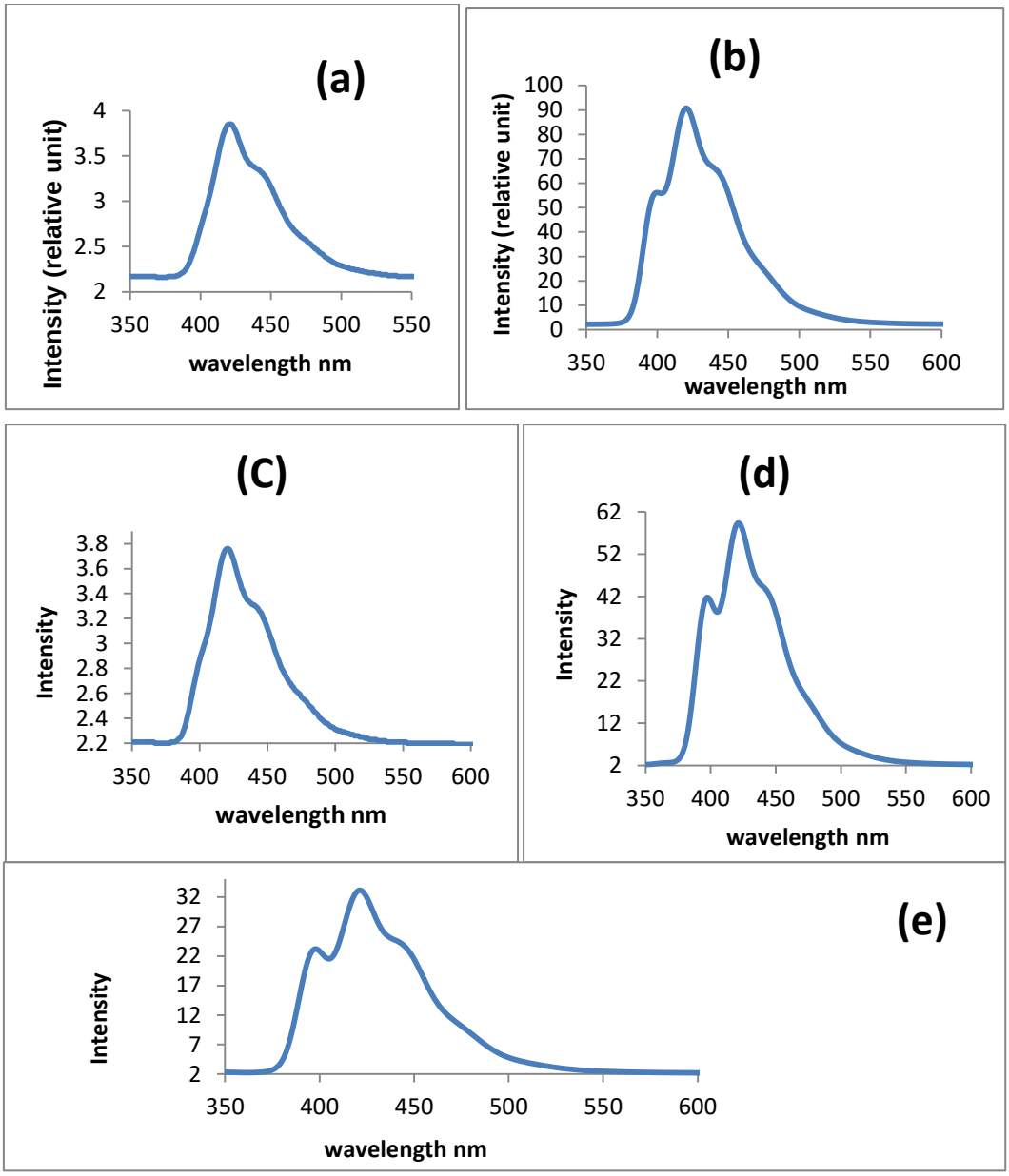

Figure 3. Fluorescence spectrum of the dye solution and popop at different concentrations: [(a) $10^{-3}\times1$, (b) 0.5×10^{-3}, (c) 1×10^{-4}, (d) 0.5×10^{-4}, (e) 1×10^{-5}] M.

It observed by the results that increase the concentration of the dye leads to displacement of fluorescence summit toward long wavelengths (Red Shift) with low-lying energies up to 60 nm.

The increase is explained by the concentration of the dye solution, the electric field Local located in the solution; will promote and thus will be re-order shipments due to electronic partial transfer where it becomes a bipolar situation irritated larger than the state of the ground; causing the polarity of the solution increase with the stability of

most of the situation irritated thus decreasing the level of energy and thus displacement of spectrum summit fluorescence site toward long wavelengths area (Red shift).[16]

Through the results of fluorescence spectra of fluorescence lifetime (τ_f) account possible as well as the Quantum Yield fluorescence (Q_f) using the relations (7) after account the area

ISSN: 2223-9944, e ISSN: 2223-9553

under the curve for curve absorption and fluorescence using a computer program (GEUP 6) The results were as shown in the table (4).

$$\tau_F = \frac{a \times \tau_{fRB}}{a_{RB}} \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (7)$$

As τ_{fRB} represents life time record for a compound which Alrodamen B and worth (3.230ns) when the concentration (10^{-4}) M and a_{RB} is the area under the curve fluorescence of rhodamine B and its value (117.6) cm^{-1} a represents the area under the curve required for the compound in this search. [17]

It can also be quantitative output of fluoridation account (Φ_F) to find the ratio of the fluorescence spectrum area to the absorption spectrum area, if any [18].

$$\phi_F = \frac{\int F(\nu)d'\nu}{\int \varepsilon(\nu)d'\nu} \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots(8)$$

$\int F(\nu)d'\nu$: The fluorescence spectrum area.

$\int \varepsilon(\nu)d'\nu$: The absorption spectrumarea.

Table 4. Fluorescence lifetime and Quantum Yield fluorescence different concentrations of dye poppop a solution

C (M)	$\tau_f(ns)x10^{-3}$	Q_f
$10^{-3}\times1$	2.90	0.5235
$10^{-3}\times0.5$	2.76	0. 5961
$10^{-4}\times1$	2.5	0.7011
$10^{-4}\times0.5$	2.19	0.8902
$10^{-5}\times1$	1.87	0.9257

It observed by the results that chronological age where they get the concentration the quantitative fluorescence output, it decreases with increasing concentration of the solution.

Theoretical Result

Theoretically and using the program (Gaussian 05) has been drawing the chemical structure of the molecule (pop pop), as well as molecular electronic orbital (HOMO) and (LUMO), her, the figure (4), figure (5), and figure (6) respectively.

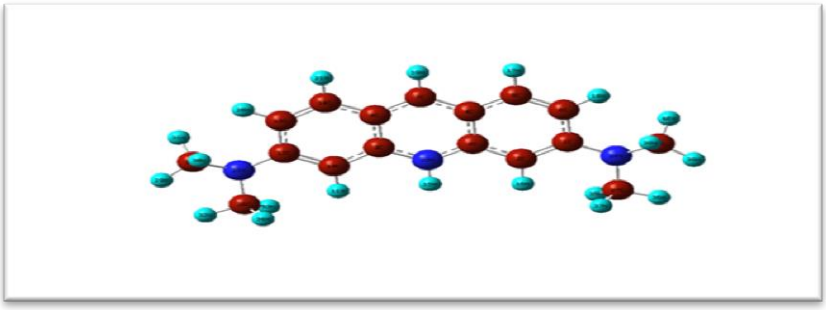

Figure 4. Chemical structure of the molecule (pop pop)

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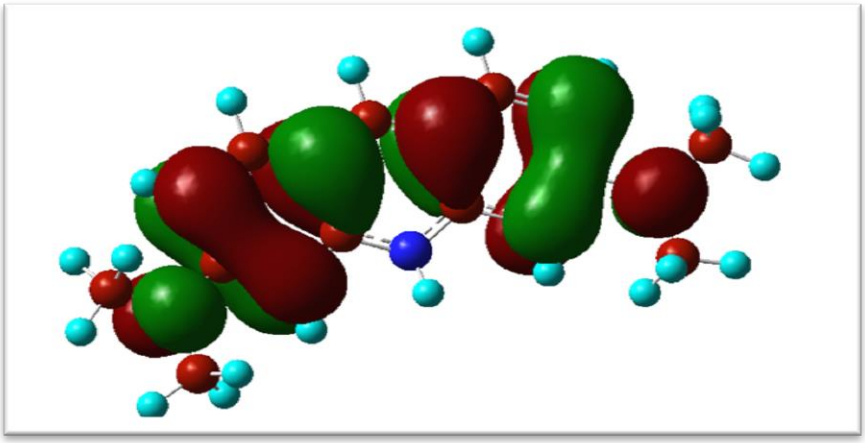

Figure 5. Molecular electronic orbital (HOMO)

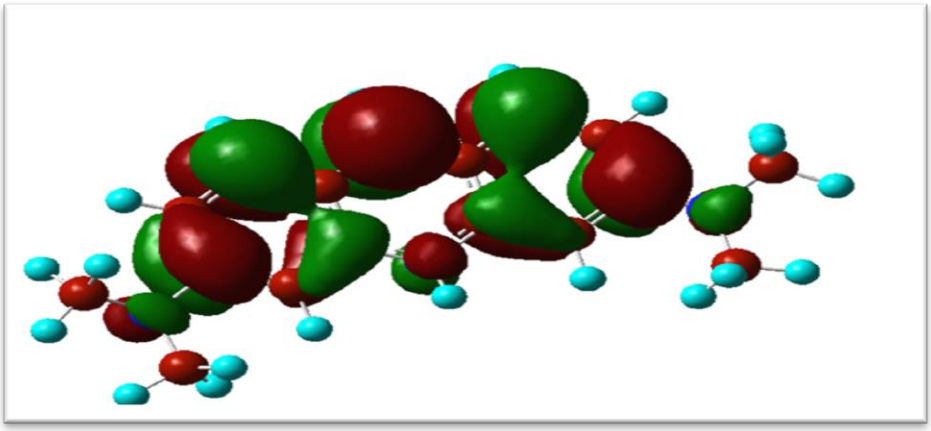

Figure 6. Molecular electronic orbital (LUMO)

DISCUSSION

Through practical results showing increased absorption intensity with concentrations so as to increase the number of molecules. The higher intensity obtained (0.983) when the concentration ($1x10^{-3}$)Ml.

The change wavelength is (blue shift) with decrease concentration, and this shows the effect of concentration on the order of the electrical energy levels in a molecule of a kind ($n \rightarrow \pi^*$).

Since the linear optical properties linked to the of absorption spectrum, we noted the effect of concentration on the absorption coefficient and reflective index.

Through fluorescence spectra possible to identify the effect of concentration on the life time and quantum yield of them.

Theoretically been identified at the molecular structure of the dye studied, it was also drawing the electrical molecular orbits. This was the kind of orbits (n, σ,σ^*,π, π^*), this relativity identical with orbital diagnosed practically.

ISSN: 2223-9944, e ISSN: 2223-9553

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ISSN: 2223-9944, e ISSN: 2223-9553