

The first steps in vision in the classroom

(Etapas iniciais para a visão na sala de aula)

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We examine, using the particle-in-the-box model, the transient absorption measurements of the cis-trans isomerization by the visual pigment rhodopsin present in the retina [R.W. Schoenlein *et al.*, Science **254**, 412 (1991)], which contains the retinene group, a conjugated system, which is formed by single and double carbon-carbon atoms, and works as a light antenna in the process of photon absorption. The present approach is directly applicable to the classroom in undergraduate chemistry and physics major courses.

Keywords: vision, quantum mechanics, undergraduate.

Analisamos, utilizando o modelo de poço de potencial infinito, o processo de absorção de um fóton que leva à isomerização cis-trans do pigmento visual rodopsina, presente na retina [R.W. Schoenlein e cols., Science **254**, 412 (1991)], que consiste de um composto formado por ligações simples e duplas entre átomos de carbono, e funciona como uma antena no processo de absorção de um fóton. A presente proposta é diretamente aplicável nos cursos de graduação em física e química, nas disciplinas de física moderna e físico-química, respectivamente.

Palavras-chave: visão, mecânica quântica, graduação.

1. Introduction

The selective absorption of light by molecules is responsible for the color of most of everyday objects, color of the eyes, the wings of butterflies, birds, vegetables, etc [1]. As opposed to most atoms and molecules, which have resonances in the ultra-violet and infrared part of the electromagnetic spectrum, the chromatic pigments as well as the photoreceptors, i.e, vision cells, contain molecules which have resonances in the visible part of the spectrum. The vision process, for pedagogical purposes, can be divided into a sequence of steps. After entering the eye, the light is focused on the retina. The photon is absorbed by the rhodopsin, and converted into a physiological message. In the case of living organisms, the optically active molecules contained in the photoreceptors consist of a dye combined with a protein, discovered by George Wald in the 1930's [2]. The molecules absorb light and transfer the absorbed energy to specific sites in order to give rise to the chemical processes. The effect of photons on rods containing molecules of rhodopsin is to convert them rapidly to molecules of retinal. From the excited state, a radiationless transition to a different configuration (isomerization). This isomerization reaction is employed as the light detection mechanism in the eye. The visible photons have energies from 1.6 eV (red) to 3.2 eV

(violet), which are low compared to normal electronic excitations, and at the same time very large compared to the molecular vibrational excitations. There exists a large number of organic pigment molecules, which have resonances in the visible, like those present in blood. The chlorophylls constitute another group of natural pigments where part of the long chain closes in a ring. They have at least two functions: they serve to absorb radiation energy as light antennae, and they are responsible for the primary process of photosynthesis in the reaction centre. In common, the organic pigment molecules, whether natural, whether synthetic, have long molecular chains constituted by single and double carbon-carbon bonds, which are known as conjugated systems [2]. One example is the rhodopsin, Greek for rose-vision, formerly known as visual purple, which is a big protein that contains the retinene group and plays a fundamental role in the absorption of light. They constitute states of large wavelength and low energy. The energy required to excite the weakly bond pi electrons, in which the magnitude of the component of the orbital angular momentum of each electron along the molecular axis is h , is relatively low, lying in the visible range. The molecules are viewed as a light antennae, or oscillators with resonance in the visible. For details about the mechanisms of seeing, the reader is referred to Refs. [3-8].

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The absorption of visible radiation by pi electrons is analog to the metallic grid which absorbs in the microwave (Fig. 1). The component of the electric field parallel to the wires accelerates the free electrons in the metal and they may move all the way up and down along the wires. In the case of the metallic grid, the energy absorbed by the electrons is converted into heat by the Joule effect, while in the case of retinal, the energy is converted into a nerve impulse in the optic nerve by the functional units surrounding the rhodopsin molecules. Humans beings cannot produce the retinal molecule in their cells [3-8]. One obtains it from the vitamin A, and the absence of this vitamin, provoke the phenomenon night blind.

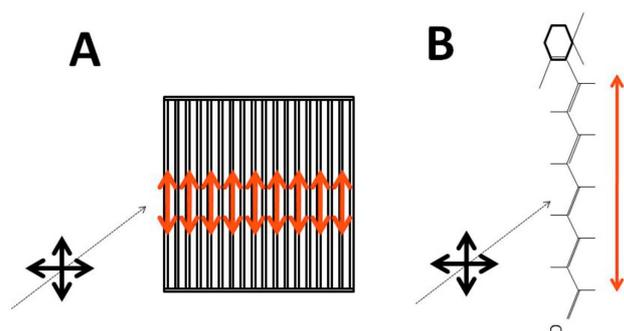


Figure 1 - The left side (A) shows the microwave absorption by a metallic grid, where the free electrons in the wires are accelerated by the parallel component of the electric field. This system is the analog of the visible photon absorption by the weakly bond non-localised pi-electrons in the retinal molecule (shown in part B), which acts as a light antennae.

In this paper, we apply a very simple model, namely the particle in a box, also known as free-electron molecular-orbital (FE-MO) method [9], in order to estimate the longest absorption wavelength of the retinene molecule. This description is behind the physical basis of the very complex mechanism of seeing. The present informal and rough approach is suitable for either introductory quantum mechanics or advanced optics courses.

1.1. The model

It is well known that a retinal rod can detect a single photon [3-6]. Vision commences when a photon is absorbed by the visual pigment and converted into electrical signals which are processed within the retina and sent to the brain. Figure 2 shows schematically the $S_0 \rightarrow S_1$ electronic vertical transition (11-cis \rightarrow 11-trans isomerization) in rhodopsin [4]. The energy difference between these two states (60 kcal/mole) corresponds to a green photon, which corroborates with the absorption curve of the main pigment in retina, the visual purple (rhodopsin), which has a maximum around 5000 Å [6].

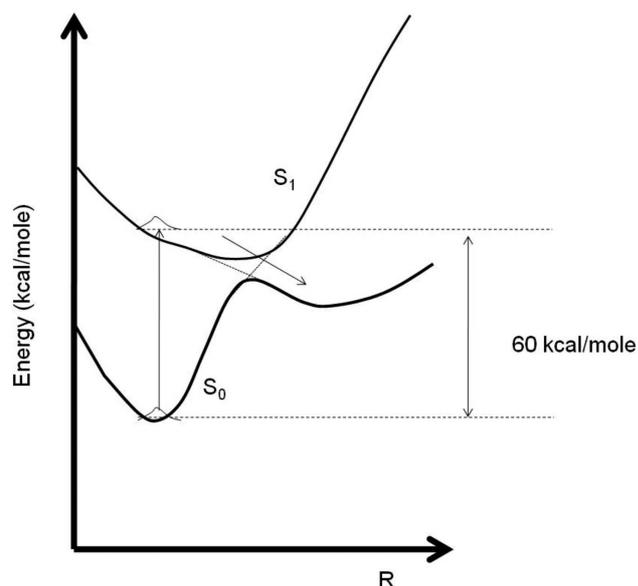


Figure 2 - Schematic ground-state singlet (S_0) and first excited-singlet state (S_1) potential energy surfaces for isomerization in rodopsin (adapted from Refs. [4] and [5]). The arrow represents the isomerization process.

Modeling medium and large molecules is a difficult task. For practical purposes, the molecular orbitals can be separated and treated distinctly in two ways, namely, the strongly bond and localised σ orbitals, and the weakly bond and delocalised π orbitals. The different symmetry characters of both orbitals, and the higher susceptibility of the pi electrons to external perturbations, such as a photon absorption, is the main justification for this approach. Many of the molecules of interest in organic chemistry have conjugated single and double carbon-carbon bonds. The alternate character of the bonds provides a kind of loosening or delocalization to the electrons. Each carbon atom contributes with one non-localised electron.

In the FE-MO method, developed in the 50's by Kuhn, Bayliss, Platt, and Simpson, the (see for instance Ref. [10] and references therein) pi electrons are treated within the independent particle model (IPM), *i.e.*, the electron-electron Coulomb correlations $1/r_{ij}$ are neglected, and the effect of the nuclei and the core electrons is represented by a particle-in-a-box potential, and the sigma orbitals will be disregarded. In general, the theoretical outcomes of this simple model is surprisingly in good agreeing with the experimental values [10].

The box, is a potential well of effective width $L = Nd$, where N is the number of carbon atoms (or pi electrons) in the active chain and d is the average distance of the C-C bond ($\sim 1,4$ Å for conjugated systems) as shown in Fig. 3. The highest filled and lowest unoccupied energy levels are pi orbitals, and play a fundamental role in the spectroscopy of the conjugated systems.

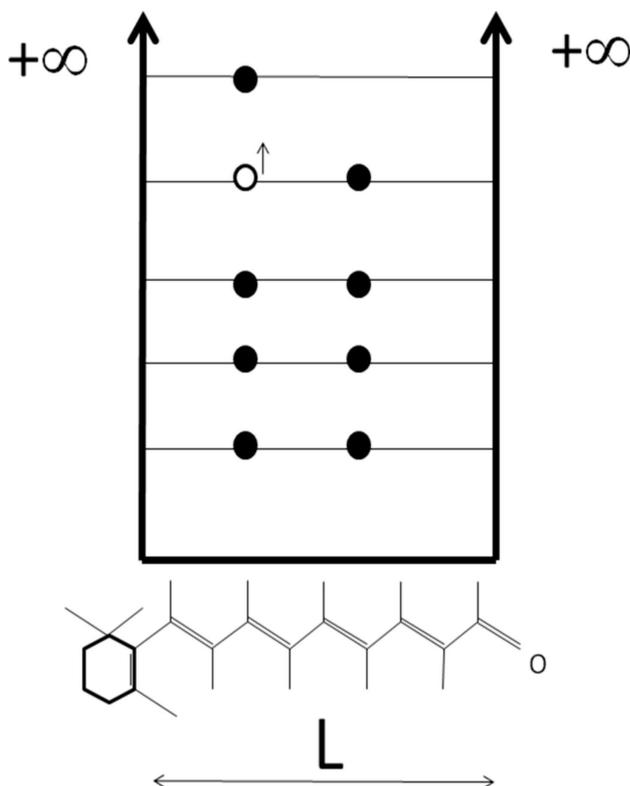


Figure 3 - The infinite potential well of width L proportional to the number of carbon atoms, where the lowest $N/2$ energy levels are filled by the N pi-electrons. The longest-wavelength electronic transition from the highest filled to the lowest unoccupied orbital is illustrated.

The Pauli principle is added in an *ad hoc* way. Each electron is put in a spin-orbital (2 electrons is a spacial molecular orbital). In the ground state, the N pi-electrons fill the first $N/2$ lowest energy levels as shown in Fig. 3.

The rod cells are sensitive to as little as one photon each. After an absorption of a photon, the molecule undergoes a electronic transition to an unoccupied orbital. The energy level of a particle of mass m in a box of width L is given by

$$E_n = \frac{h^2 n^2}{8mL^2}. \quad (1)$$

The selection rule for the infinite potential well allows the quantum number n to change by an odd integer [10]. The energy absorbed in the transition n to $n + 1$ is given by

$$\Delta E = E_{n+1} - E_n = \frac{h^2(2n+1)}{8mL^2}. \quad (2)$$

As mentioned above, the N pi-electrons, fill the $n = N/2$ lowest energy levels. Then, using the above assumptions, we have

$$\Delta E = \frac{h^2(N+1)}{8md^2N^2} = 19,2 \frac{(N+1)}{N^2} \text{ eV}. \quad (3)$$

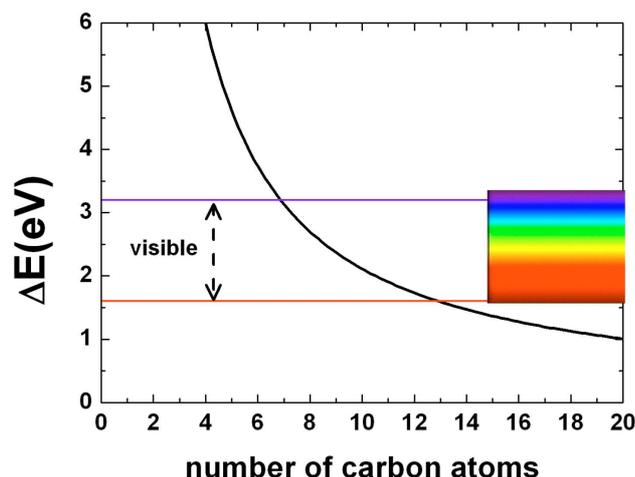


Figure 4 - The energy acquired by a conjugated system after an absorption of a photon, corresponding to the longest-wavelength electronic transition (Eq. (3)), ΔE in eV, as a function of the effective number of carbon atoms in the chain. For display purposes, ΔE is plotted as a continuum function. The horizontal lines represent the visible part of the electromagnetic spectrum (1.6-3.2 eV). The corresponding photon wavelengths can be calculated using $\lambda(\text{\AA}) = 12398/E(\text{eV})$.

For the case of the retinal molecule, illustrated in Figs. 3 and 4, if one assumes that the effective length L , of the optically active part of the molecule is 12,6 \AA or 9 carbon atoms, the transition energy is ~ 2.5 eV. This is in agreement with the $S_0 \rightarrow S_1$ electronic transition (11-cis \rightarrow 11-trans isomerization) in rhodopsin [4, 5]. This energy corresponds to a green photon, which corroborates with the absorption curve of the main pigment in retina, the visual purple (rhodopsin), which has a maximum around 5000 \AA [6].

From Eq. (3) and Fig. 4 we see that, in this naïve model, the electronic energy levels, and then the spectral sensitivity depend strongly on the effective number of carbons atoms in the chain. For large N , the transition energy goes as $\sim 1/N$. The spectral sensitivity is controlled by a combination the amino acid sequence of the opsin. By performing small structural modifications in the molecule, changing the width of the well for instance, the absorption spectrum can be shifted. Living organisms make use of this fact when they exist under conditions where the light has a diferent spectral composition than that of normal sunlight. Color depends on the light intensity. For a very interesting description of color vision and the mechanisms os seeing, the reader is referred to chapters 35 and 36 of Ref. [6].

1.2. Summary

The infinite potential well was applied to study in order to obtain robust estimates of the longest wavelength transition of the retinal molecule, the main group contained in the most common retina pigment. This simple model takes account the physical basis of the complex mechanism of seeing. The predicted transition energies corresponding to the longest-wavelength for the retinal

molecule corroborates with the absorption curve of the main pigment in retina, the visual purple (rhodopsin), which has a maximum around 5000 Å. The rigor in exposition was sacrificed in the benefit of a consistent account of the physical basis of the vision process.

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