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Struture of Matter

Chapter 5: Molecules

Book Reference: Alonso e Fin - Quantum and Statistical Physics

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Exercise 5.25:

The β-carotene molecule is a conjugated molecule having 22 π -electrons. It has been found that this molecule shows strong absorption of radiation at 4510Å. Estimate the total lenght of the molecule.

Soluction

The β-caroteno molecule, can be represented by the Fig.1).

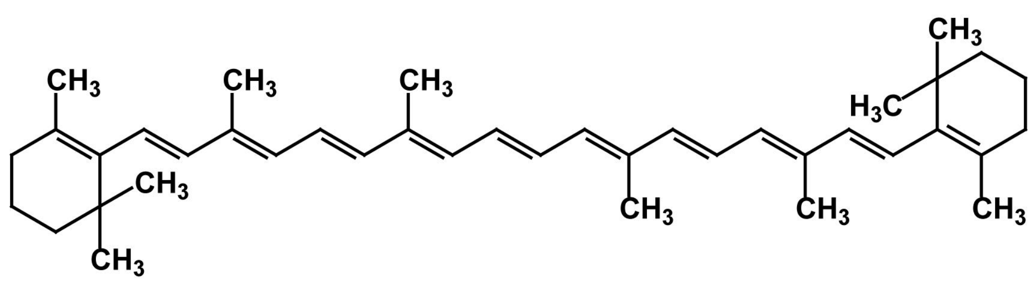

Figure 1: Struture of β-caroteno Molecular

We know that the energy of a particle is

$$E = \frac{p^2}{2m} \tag{1}$$

in a potencial box, the momentum can be write

$$p = \hbar k = \frac{n\pi\hbar}{a} \quad \therefore \quad k = \frac{n\pi}{a} \tag{2}$$

so is possible rewrite the energy by

$$E_n = \frac{n^2\pi^2\hbar^2}{2ma^2} \tag{3}$$

For the transition of n to $(n+1)$,

$$\Delta E = E_{n+1} - E_n \tag{4}$$

$$= \frac{(n+1)^2\pi^2\hbar^2}{2ma^2} - \frac{n^2\pi^2\hbar^2}{2ma^2} \tag{5}$$

$$= \frac{\pi^2\hbar^2}{2ma^2}\left[(n+1)^2 - n^2\right] \tag{6}$$

$$= \frac{\pi^2\hbar^2}{2ma^2}\left[n^2 + 1 + 2n - n^2\right] \tag{7}$$

So, we can rewrite the energy between the nth and $(n+1)$th levels is the first excitation energy, that corresponds the strong absorption of radiation.

$$\Delta E = \frac{(2n+1)\pi^2\hbar^2}{2ma^2} \tag{8}$$

$$\Delta E = \frac{h^2(2n+1)}{8ma^2} \quad , \quad \hbar = \frac{h}{2\pi} \tag{9}$$

Where the a is the lenght of t he region in which the π-electrons move, taken as the molecular lenght extended half a bond lenght on each end, and de m is the molecular mass.

So, being the molecular mass of the β-carotene is $m_\beta = 5.817\text{x}10^{-12}$[Kg], and by the lenght of the radiation $\lambda = 4510\text{Å}$, is possible describe the difference of energy by the transition state.

$$\Delta E = h\nu = \frac{hc}{\lambda} \tag{10}$$

With the Eq.(9), we can write the lenght a

$$a = \sqrt{\frac{h^2(2n+1)}{8m_\beta \Delta E}} \tag{11}$$

$$
\begin{aligned}
a &= \sqrt{\frac{h^2(2n+1)}{8m_\beta \frac{hc}{\lambda}}} \qquad (12)\\
a &= \sqrt{\frac{h\lambda(2n+1)}{8m_\beta c}} \qquad (13)
\end{aligned}
$$

If the β-carotene chain has $2n$ atoms, there are $2n$ π-electrons and the last occupied electronic level corresponds to nth level. As we have the $n = 11$, corresponding of 22π-electrons of the β-caroteno.

Calculate the Eq.(13), with the values that we have,

$$
\begin{aligned}
h &= 4.13566743 \times 10^{-15}\ [eV] \qquad (14)\\
c &= 2.99792458 \times 10^{8}\ [m/s^2] \qquad (15)\\
\lambda &= 4510 \times 10^{-10}[m] \qquad (16)
\end{aligned}
$$

so resolving the Eq.(13), we obtain the lenght of the β-caroteno molecule

$$
a = 1.77 \times 10^{-9} \qquad (17)
$$

equivalent of a $=$ 17.7Å.