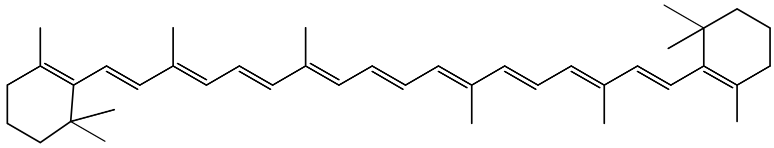
**Fisicoquímica de Biomoléculas 2006/2007. Hoja 1**
**Área de Química-Física. Universidad Pablo de Olavide**



**1.- β-carotene's orange color:** β-carotene is a linear poliene with 21 conjugated bonds, 10 single and 11 double bonds in alternating order. Assume for this exercise that the C-C bond distance is 140 pm. By using the particle-in-a-box theory, determine the wavelength of the radiation required to induce an electronic transition from level 11 to 12 in the β-carotene molecule. Compare and discuss the calculated wavelength with the experimental value.
**Data:** $h=6.6\times10^{-34}$ Js; $m_e=9.1\times10^{-31}$ kg; Velocidad de la luz: $3\times10^{8}$ $ms^{-1}$. Experimentally, absorbance is peaked at 497 nm.

**2.- Degenerate energy levels:** Consider a particle in a three dimensional box of side lengths $L_x$, $L_y$, $L_z$ such that $L_x=L_y\neq L_z$. Construct a table contemplating all possible values of $n_x$, $n_y$, $n_z$, with quantum numbers up to 3 and the associated energies. Deduce from it the degeneracies of the levels. Given that the values of $n$ can be arbitrarily big, ¿from which energy on is it necessary to probe values of $n$ above 3 to be sure that the degeneracy found so far is the correct one? Assume for this exercise that $L_x^2 / L_z^2 = 2$.

**3.- Vibration of the N-H bond in the peptide binding. Effect of neglecting the heavy atom movement:** We want to study the fundamental vibrational state of the N-H bond, considering it to behave like a harmonic oscillator. The force constant for the N-H bond is found to be 300 $Nm^{-1}$ and the hydrogen atom mass is $m = 1.67\times10^{-27}$ Kg.
a) in this first part, consider that the N atom is fixed. Calculate the vibrational frequency (in $s^{-1}$) and convert it to a wavenumber (in $cm^{-1}$).
b) Repeat the frequency calculation as if the bond corresponded to a diatomic molecule. ¿Express the change as a percentage of the case treated in a?
c) Calculate the separation in energies between vibrational levels in the case a. Estimate the amplitude of the vibration of the fundamental vibration (based on a classical description).
**Data:** $h=6.6\times10^{-34}$ Js

**4.-Isotopic effect:** Calculate the fundamental vibrational frequency of carbon monoxide, CO, considering it to behave like a harmonic oscillator with a force constant 1902.5 N $m^{-1}$. By how much will this frequency change if the molecule contains the isotope $^{13}C$ instead of the more abundant $^{12}C$?

**5.-Macroscopic systems are in high quantum states:** A 45 g mass attached to a spring whose other end is fixed oscillates at a frequency of 2.4 vibrations per second, with an amplitude of 4.0 cm. Calculate the force constant of the spring. What would the quantum number $n$ be if the system were to be treated quantum mechanically?
**Data:** $h=6.6\times10^{-34}$ Js

**6.-Reactive oxygen species:** In some metabolic processes electrons escape and are captured by molecular oxygen converting it in the very reactive superoxide ion that must be converted in controlled manner to a less reactive species. Under the action of the superoxide dismutase enzyme, the superoxide ion is dismutated in oxygen peroxide, a strong oxidant, and $O_2$. The next step consists in the dismutation of oxygen peroxide to form water and $O_2$, performed by catalases and peroxidases.
Write down the sequence of reactions described. Give the oxidation states of the different oxygen species mentionned. Sketch the molecular orbital diagram of $O_2$, and of the $O_2^-$ species (superoxide ion). Say whether they are radicals and what are their bond orders.