

Research Paper :

Spectral analysis and effect of temperature on thermodynamic parameters and biological activities of some substituted quinoline

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ABSTRACT

The present paper concerns with an introduction of the molecular spectroscopy in brief, selection rule for infrared, Raman spectra and electronic transition. Electronic and vibrational spectra of benzene and quinoline substituents have been discussed. The present paper also concerns the effect of substituents, their position on the vibrational and electronic spectra and the effect of polar and nonpolar solvents have also been discussed. The present investigation also concerns the effect of pH on the vibrational and electronic spectra have also been discussed. The subject also concerns Thermodynamic parameters and biological studies have also been discussed.

KEY WORDS : Infrared spectra, Raman spectra, Electronic and vibrational spectra of quinolines substituents

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When a molecule absorbs its energy increases in proportion to the energy of the photon as expressed by the relation:

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

where, h is Planck's constant, ν' and λ are the frequency and the wavelength of radiation and c the velocity of light. The increase may be in the form of electronic, vibrational and rotational energy of the molecule. Changes in the electronic energy involves relatively large quanta, while in the vibrational energy involve smaller quanta and the change in the rotational energy involves even smaller than those of vibrational energy. If a molecule absorbs radiation in the microwave or far infrared region, only its rotational energy will change. If the energy of the radiation is much greater, as in the case of ultra-violet light, there will be a change in the electronic, vibrational and rotational energies of the molecule. Thus the infrared absorption spectra of the molecules result from transition between vibrational and rotational energy levels. In conclusion, molecular spectroscopy is the study of the absorption or emission of electro-magnetic radiation by the molecules. The spectral regions, infrared, visible and ultra-violet are classified from 0.8 microns to 1000 microns, from 400

nm to 800nm, from 1 nm to 400 nm, respectively. The modes which involve a change of dipole moment during vibration will yield infrared bands, while change in the polarizability may give to Raman bands and the modes which neither involve a change in dipole moment nor in polarizability may appear in the electronic spectra. Although the mechanism of absorption of energy is different in the ultra-violet, visible and infrared region, the fundamental process is the absorption of a certain amount of energy which provide complete information about the vibrational frequencies of the molecule in the ground and excited electronic states^{1,2}.

If a molecule is placed in an electromagnetic field, a transfer of energy from the field to the molecule will occur only when the difference of the energy E between two quantized states as given below:

$$\Delta E = h\nu = E_2 - E_1$$

where, h is the Planck's constant, and ν is the frequency of radiation. These transitions (E_1 to E_2 , absorption or E_2 to E_1 , emission) involve different amount of energy.

The nature of the molecular changes that are responsible for the emission or absorption of the radiation can be easily understood with advanced experimental techniques to a high degree of accuracy. The experimental