Application of spectroscopic methods in molecular structure determination

Assignment 1 on module 1 – General aspects of spectroscopic methods

Fundamental constants useful for calculations:

Speed of light = c = 3.0 x 108 ms^{-1}, Planck's constant = h = 6.626 x 10^{-34} Js and h/2π = 1.055 x 10^{-34} Js

Avogadro number = N = 6.022 x 10^{23} mol^{-1}, Boltzmann constant = k = 1.381 x 10^{-23} JK^{-1}

1 eV = 1.602 x 10^{-19} J *and* 1 wavenumber (cm^{-1}) = 1.986 x 10^{-23} J

1. Raman spectroscopy is a absorption/emission/scatter spectroscopy. (Choose the correct answer).

2. In vibrational spectroscopy it is the electric field vector/magnetic field vector of the electromagnetic radiation that interacts with the molecules during vibrational excitation. (Choose the correct answer).

3. Name a spectroscopic method that uses 600 MHz frequency of radiation as the excitation source. Which region of the electromagnetic radiation is this frequency correspond to?

4. Calculate energy per photon and energy per mole of photons of light of wavelength 250 nm and another light of frequency 500 MHz. Report the values in eV and Joules mol^{-1}, respectively.

5. If the FWHM of an infrared spectral line is 2000 cm^{-1}, calculate the life time of the excited state.

6. The energy gap (ΔE) between two electronic energy levels is 2.5 eV in a molecule. Calculate the population ratio of molecules in excited state to the ground state (N_{ex}/N_{gr}) of this electronic level at 25 ^{o}C using Maxwell-Boltzmann distribution.

7. Among vibrational spectroscopy, UV-Vis spectroscopy, rotational spectroscopy and NMR spectroscopy arrange them in the increasing order of sensitivity purely based on excess population of the ground state with respect to the corresponding excited state. State reasons for your answer.

8. Calculate the concentration of a solution which has molar absorptivity of 2.0 x 10^{5} L mol^{-1} cm^{-1} at 500 nm with an absorbance of 0.4.

9. Two peaks appeared at δ 2.0 ppm and 2.2 ppm in the NMR spectrum of a compound. Calculate their chemical shift values in Hz in a 60 MHz instrument and in a 600 MHz instrument.

10. ^{1}H NMR spectrum of a mixture containing *o*-nitrotoluene and *p*-nitrotoluene showed two peaks for the methyl group in these compounds. The methyl peak of *o*-nitrotoluene appeared at d 2.5 ppm with an integration (area under the peak) of 52 and the methyl peak of *p*-nitrotoluene appeared at d 2.3 ppm with an integration of 28. Calculate the mole ratio of these two compounds in the mixture.