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ACA-3881 Seat No._____

M. Sc. (Sem. II) Examination

March / April - 2019

Chemistry : CHN - 504 (A)

(Spectroscopy)

Time : 2 Hours] [Total Marks : 50

1 Answer any **five** : 20

(a) Discuss the statement for the vibration of a diatomic molecule, the energy difference between successive vibrational levels is $\bar{v}\ cm^{-1}$ and hence vibrational levels are equally spaced.

(b) Explain vibrations of Polyatomic molecules. Write likely modes of vibrations of the formate ion.

(c) On the basis of relative values of principal moments of inertia classify the molecules.

(d) Describe Excess Population and Saturation in relation to population densities of nuclear spin states.

(e) Define with schematic diagram :

(i) Diamagnetic anisotropy

(ii) Delta (δ) unit

(iii) Chemical shift

(iv) Local diamagnetic current.

(f) Give a Physical picture of spin-spin coupling for one bond couplings $\left({}^{1}J\right)$ and two bond couplings $\left({}^{2}J\right)$.

(g) Define with suitable illustration following terms in relation to Raman Spectroscopy:

(i) Rayleigh scattering

(ii) Stokes and anti-Stokes lines.

(h) For Rotational spectra of rigid diatomic molecules, derive an expression, the frequency of the absorption line is given by : $\overline{v}_j = 2B(J+1)cm^{-1}$, $J = 0,1,2...$

2 Answer any **five** : **20**

(a) How Overtone and combination bands and Fermi Resonance complicate Infrared spectrum?

(b) The equilibrium frequency of $^{12}C^{16}O$ corresponds to $2143\,cm^{-1}$. Calculate the frequency of $^{13}C^{16}O$ using integer mass numbers.

(c) Show schematically First order Stark Effect of a symmetric top molecule for the $J = 1, K1 \rightarrow J = 2, K = 1$ transition. List out the importance of Stark effect.

(d) Define : First order and second order Spectra. Discuss splitting patterns in AMX Spin systems.

(e) Give brief account on the Continuous Wave (CW) Instrument.

(f) If the bond length of H_2 is $0.07417\ nm$, what would be the positions of the first three rotational Raman lines in the spectrum? What is the effect of nuclear spin on the Spectrum? $1\ H = 1.673 \times 10^{-27}\ kg$.

(g) Explain the principle of Mutual Exclusion with example.

(h) Why anti-Stokes lines are less intense than Stokes lines?

3 Answer any **five** questions in brief : **10**

(a) What is Quadrupole Hyperfine Interaction? Illustrate with suitable examples.

(b) Explicate Fermi Resonance and Overtone and combination band.

(c) Give brief account on ^{31}P resonance spectra.

(d) Define Pulse; Time domain signal; Frequency domain signal and noise in NMR Spectroscopy.

(e) How Double Resonance is used to simplify NMR Spectra ? Explain application of spin decoupling for Propyl bromide molecule.

(f) Write important applications of FT-NMR in medical diagnostics.

(g) Give account on Quantum Theory of Raman Effect.

(h) Explain selection rule for energy transition for the Raman Scattering. Show that the frequency of the Raman lines will be $\overline{\nu}_{Raman} = \overline{\nu}_{ex} \pm \overline{\nu}_{e}$.