MANIPAL
ACADEMY of HIGHER EDUCATION
(Deemed to be University under Section 3 of the UGC Act, 1956)

DEPARTMENT OF SCIENCES, I SEMESTER M.Sc. (CHEMISTRY)
END SEMESTER EXAMINATIONS, Feb 2022

Subject: Spectroscopy – I [CHM5104]

(Choice-Based Credit System, 2020)

Time: 2 Hours Date: 14 Feb. 2022 MAX. MARKS: 40

Note: answer any four questions.

1 A. Discuss the rotational spectrum of rigid and non-rigid diatomic molecule. Write any two consequences of elasticity of the bond in the microwave spectroscopy.

1 B. Show that spectral lines are equally spaced in the vibrational spectrum of a simple harmonic diatomic molecule. Calculate the approximate wave number of the fundamental absorption peak due to the stretching vibrations of a HCl molecule. The force constant for H-Cl bond has an approximate value of 2×10^6 dynes/cm. The atomic masses are: H= 1.673×10^{-27} kg and Cl = 58.06×10^{-27} kg.

1 C. State and deduce Beer's law. Calculate the energy (in joules and in eV) of CO molecule in the second excited rotational level, if the inter-nuclear distance of molecule is 0.113 nm. The atomic masses are $^{12}C=1.99\times10^{-26}$ kg; $^{16}O = 2.66\times10^{-26}$ kg

(3 + 3+ 4)

2A. Give reason for the following;

i) Aniline shows blue shift in the acidic medium.

ii) Ordinary glass cuvettes can't be used for recording UV spectrum

iii) Water is used as a solvent in Raman spectroscopy

2B. Differentiate between the following;

i) Dispersive and FTIR instruments

ii) $\sigma \rightarrow \sigma^*$ and $\pi \rightarrow \pi^*$ electronic transitions

iii) Qualitative and quantitative methods of analysis

2C. Describe the Woodward Fiesher rules for homo/hetero annular dienes in UV-Visible spectroscopy and Calculate the λ_{max} for 1, 4-dimenthyl cyclohex-1,3-diene.

(3+3+4)

3A. Describe the Quantum theory of Raman spectroscopy and write two differences between Stoke's and Anti-stoke's line.

3B. Describe the theory of vibrational Raman spectroscopy and calculate the bond distance of H_2 molecule if the rotational Raman spectrum of H_2 gas is found to consist of a series of Stokes and antistokes lines, the first of which appears at 345.9 cm-1 relative to the source of excitation. Given. The atomic mass of hydrogen atom is 1.68×10^{-27} kg.

3C. Explain the procedure for the quantitative determination of lead present in a sample of water through Atomic Absorption Spectroscopy. Mention two differences between Atomic Absorption Spectroscopy and Flame Photometry.

(3 + 3+4)

4A. Describe the interaction of X-ray and radiofrequency region of the electromagnetic spectrum with the organic molecules. Discuss any one factor influencing the intensity of spectral lines.

4B. Describe the following in Atomic Absorption Spectroscopy.

i) Solvent Interference
ii) Continuous Deuterium source
iii) Carbon atomizers

4C. Explain the factors responsible for the width of spectral lines. List all the symmetry operations that can be carried on NH_3.

(3+3+4)

5A. Explain with an example the identification of molecules possessing permanent dipole moment based on the symmetry aspects of a molecule. What is meant by a point group? Why is horizontal mirror plane not possible on H_2O?

5B. Give reasons for the following:

(i) Symmetry operations of water molecule forms an Abelian group
(ii) Controlling the flame temperatures is crucial in flame photometry.
(iii) Chopper is interposed between the hollow cathode lamp and flame in Atomic Absorption Spectroscopy.

5C. Determine the point group of the given molecules by following the systematic procedure.

i) PCl_3
ii) $[PtCl_4]^{2-}$
iii) Staggered ferrocene
iv) HCl

(3+3+4)

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