LOYOLA COLLEGE (AUTONOMOUS), CHENNAI - 600 034

M.Sc. DEGREE EXAMINATION – PHYSICS

THIRD SEMESTER - NOVEMBER 2018

16/17PPH3MC02/PH 3815 - SPECTROSCOPY

Date: 27-10-2018 Dept. No. Time: 09:00-12:00

PART – A

 $(10 \times 2 = 20)$

Max.: 100 Marks

- 1. Distinguish between symmetric top, spherical top and asymmetric top molecules.
- 2. What are hot bands? Why are they so called?
- 3. The fundamental vibration frequency of HCl is 2989 cm⁻¹. Find the force constant of the HCl bond.
- 4. In H₂ molecule the separation between adjacent rotational Raman lines is 4B whereas in O₂ it is 8B. Why?
- 5. Theg_N value for F^{19} nucleus is 5.256. Calculate resonance frequency when it is placed in a magnetic field of strength 1.2 T and β_N is $5.0504 \times 10^{-27} \text{ JT}^{-1}$
- 6. What are the advantages of TMS in NMR spectroscopy?
- 7. What is pre-dissociation?
- 8. Calculate the ESR frequency of a free electron in a magnetic field of strength 2.5 T. Given that g =2.0023 and $\mu_B = 9.274 \times 10^{-24} \text{ JT}^{-1}$.
- 9. Write any two applications of SEM.
- 10. What is the principle of AFM?

PART - B

Answer ANY FOUR questions

- 11. Derive an expression for the Moment of Inertia of OCS molecule, in terms of the bond length. Also, explain how the bond lengths can be found by isotopic substitution method.
- 12. (a) Explain the polarizability ellipsoid. On the basis of polarizability, outline the vibrational Raman Effect of H₂O. (5)

(b) If the bond length of H_2 is 0.07417 nm, what would be the positions of the first three rotational (2.5)Raman lines in the spectrum?

- 13. Explain the vibration spectrum of a diatomic molecule. Deduce the effect of anharmonicity.
- 14. Draw the schematic diagram of NMR spectrometer and explain its functioning.
- 15. Explain dissociation energy in detail.
- 16. Discuss Reflection Absorption Spectroscopy.



Answer all questions

 $(4 \times 7.5 = 30)$

$\underline{PART - C}$

Answer ANY FOUR questions $(4 \times 12.5 = 50)$ 17. (a) Explain with theory, the spectrum of symmetric top molecule. (8) (b) The three consecutive lines in the rotational spectrum of HBr are 84.544, 101.355 and 118.112 cm⁻¹. Find the values of rotational constant, centrifugal distortion constant and vibrational frequency. (4.5)18. Explain the theory of pure rotational Raman spectra of (i) Linear molecule (ii) Symmetric top molecule. 19. (a) Explain the principle and instrumentation of Mossbauer Spectroscopy. (10) (b) An excited ⁵⁷Fe* nucleus, recoiling at 10^2 m/s emits γ -radiation with frequency 3.2×10^{18} Hz. Calculate the Doppler shift in γ -ray frequency. (2.5)20. State Franck-Condon principle. Account for intensity of spectral lines and explain why the spectrum is discrete and not continuous. 21. Describe the functioning of PES and XPES. 22. (a) What is Fortrat parabola? Obtain expression for band head. (5.5)

(b) Explain chemical shift in NMR. (7)

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