MAHATMA GANDHI UNIVERSITY

CBCSS B.Sc PROGRAMME IN CHEMISTRY

Fifth Semester

Core Course :CH5B04 – Quantum Mechanics and Spectroscopy

Model Question Paper

Time: Three hours Total weightage: 25

Section A
(Answer all questions. Each bunch of four questions carries a weightage of 1)

I. *Fill up the blanks*
1. Davisson and Germer experiment illustrates ---------- nature of electron
2. A 3p orbital has ---------- radial nodes
3. The frequencies of radiations emitted in fluorescence are ----- than that of the incident radiation
4. A diatomic molecule executing simple harmonic oscillation obeys ------ law

II
5. How many signals are there in the PMR spectrum of neopentane?
6. A compound shows a PMR peak at 240Hz downfield from the TMS peak in a spectrometer operating at 60MHz.What is the chemical shift in ppm?
7. Which among the following molecule is IR inactive but Raman active?
   (a) HCl; (b) N_2; (c) SO_2; (d) CH_4
8. Name the spectroscopic technique used in molecular mass determination.

III
9. What is commutator operator?
10. Which among the following is a chromophore?
    --OH ; -N=N- ; NH_2 ; OR
11. Which absorbs at higher frequency,OH or CO group?.
12. What is the range of frequencies covered by pure rotational spectra?.

IV State whether the following statements are true or false
13. Schrodinger equation is an eigen value equation
14. Comption effect illustrates the wave nature of light
15. Non-polar molecules are microwave active
16. The number of bands in the IR Spectrum of a molecule is the same as the number of normal modes of vibration (4x1= 4)

Section B
(Answer any 5 questions. Each carries a weightage of 1)

17. Describe the features of black body radiation
18. What is ψ^2 ? What is its physical meaning?
19. Differentiate between fundamental and overtone transitions
20. What are the advantages of using TMS as a reference in NMR spectroscopy?
21. Why is it that in the excited state of a molecule the vibrational frequency is smaller than in the ground state?

22. Give any four experiments which showed the inadequacy of classical mechanics
23. What is Born-Oppenheimer approximation? Explain
24. How is mass spectrum of a compound obtained? Explain (5x1=5)

Section C
(Answer any 4 questions. Each carries a weightage of 2)

25. Explain chemical shift in NMR. Why is chemical shift expressed in ppm?
26. State and explain the Franck-Condon principle
27. Calculate the frequency of light emitted when an electron jumps from the first excited state of butadiene to its ground state using particle in a box approximation. Given that the length of the carbon chain in butadiene is 578 pm
28. Compare and contrast σ, σ^*, π, and π^* molecular orbitals
29. The microwave spectrum of HCl consists of a series of equally spaced lines separated by 20.86 cm^{-1}.Calculate the bond length of HCl
30. State and explain Einstein law of photochemical equivalence. What is meant by quantum yield of a photochemical reaction? (4x2=8)

Section D
(Answer any two questions. Each carries a weightage of 4)

31. State and explain the postulates of quantum mechanics
32. (a) Discuss the principles of NMR spectroscopy
    (b) Explain spin-spin splitting in NMR
33. (a) Briefly explain the quantum theory of Raman effect
    (c) If HCl is irradiated with 435.8nm mercury line calculate the Raman line in nm if the fundamental vibrational frequency of HCl is 8.667×10^{13} s^{-1}

(2x4=8)
