

M.Sc. (Chemistry) Sem- II
Question Bank-CHP-4201-Fundamentals of Physical Chemistry-II

SECTION-I

A) Multiple choice question

1. On which factors the vibrational stretching frequencies of diatomic molecule depend?
 - a) Force constant
 - b) Atomic population
 - c) Temperature
 - d) Magnetic field
2. Since the nuclei in a polyatomic molecule do not always vibrate in a simple harmonic manner, there arises one of the following situations?
 - a) Harmonicity
 - b) Anharmonicity in molecular vibrations
 - c) Fundamental frequencies
 - d) All of the above
3. What is order of decreasing vibrational frequency for C-Cl, C-Br, C-C, C-O, C-H
 - a) C-H, C-C, C-O, C-Cl, C-Br
 - b) C-Cl, C-Br, C-C, C-H, C-O
 - c) C-Cl, C-H, C-C, C-O, C-Br
 - d) C-Cl, C-Br, C-C, C-O, C-H
4. In IR spectroscopy which frequency range is known as the fingerprint region?
 - a) $400-1400\text{cm}^{-1}$
 - b) $1400-900\text{cm}^{-1}$
 - c) $900-600\text{cm}^{-1}$
 - d) $600-250\text{cm}^{-1}$
5. Chemical shifts originates from-
 - a) Magnetic momentum
 - b) Electron shielding
 - c) Free induction decay
 - d) Scalar coupling
6. Which of the following transitions are of weak intensities and lie in the visible region?
 - a) $n-n^*$
 - b) $\sigma-\sigma^*$
 - c) $\Pi-\Pi^*$
 - d) $n-\sigma^*$
7. Which of the following shift leads to the decreased intensity of absorption?
 - a) Hypochromic
 - b) Hyper chromic
 - c) Hypochromic
 - d) Bathochromic

8. Which of the following is an application of electronic spectroscopy?
- Detection of impurities
 - Control of purification
 - Study of kinetics of the chemical reaction
 - All of the above
9. The microwave active molecules are-
- HCl, OCS
 - C0,CO₂
 - Both a) and b)
 - None of the above
10. Selection rule for Raman spectroscopy-
- $\Delta J = \pm 1$
 - $\Delta J = 0, \pm 1, \pm 2, \dots$
 - $\Delta J = \pm 2$
 - $\Delta J = 0$

B) One sentence answer

- Write a definition of spectroscopy?
- Enlist different regions of electromagnetic spectrum.
- What is mean by zero point energy?
- Define the terms frequency and wavelength.
- Write down one example of symmetric top and spherical top molecules.
- Why N₂ molecule is inactive to rotational spectroscopy?
- Give the equations of fundamental absorption and first overtone.
- Write down the rule of mutual exclusion.
- What are the Stokes lines and antistokes lines?
- Write down the Stark effect.
- Define and explain predissociation.
- Write down Born-Oppenheimer approximation.
- Give the equation of Rotational constant and moment of inertia.
- Write down the applications of microwave spectroscopy.
- Define the term plane polarized light.

C) Short notes

- Write a short note on predissociation
- Write a short note on factors affecting width of spectral lines.
- Write a short note on factors affecting intensity of spectral lines.
- Write in short applications of Raman spectroscopy.
11. Explain I short 'electronic spectra of diatomic molecules'.
12. Write down radiometric titrations.
13. Write down Frank-Condon principle
14. Write down the applications of electronic spectroscopy.
15. Write in short chemical applications of ¹H-NMR.
16. Write in short applications of ESR and Mossbauer spectroscopy

17. Write a note on polarization of light and Raman effect
18. Write a note on Vibrational coarse structure.
19. Write a note on Birge- Sponer extrapolation.
20. Write a short note on coarse and fine structure.
21. Write a note on Frank- Condon principle.
22. Give the classification of rigid rotors.
23. Write a note on transitions observed in the rotational spectrum.
24. Define degeneracy and explain it in detail for energy levels $J=1$ and $J=2$.
25. Write down the effect of isotopic substitution on the spectrum of carbon monoxide.

D) Short answer questions

1. Discuss the principle of IR spectroscopy in the molecular structure elucidation.
2. Write down the rule of mutual exclusion in Raman spectroscopy..
3. Define and explain predissociation.
4. State Frank-Condon principle.
5. Discuss the general rules governing the number of lines observed in ESR spectroscopy.
6. Sketch and explain Fortrat diagram.
7. Describe in brief rotational fine structure of electronic-vibration transitions.
8. Explain quantum theory and classical theory of Raman effect.
9. Write down the rule of mutual exclusion.
10. Explain Stokes and antistokes lines.
11. Define and explain predissociation.
12. State Frank-Condon principle.
13. Write down selection rule for pure rotational Raman activity in linear molecules.
14. Explain factors determining the intensity of spectral lines.
15. Describe in brief rotational fine structure of electronic-vibration transitions.
16. Explain simple harmonic oscillator and anharmonic oscillator and give selection rules.
17. Why is the selection rule for pure rotational Raman spectrum is $\Delta J = \pm 2$ and $\Delta J = \pm 1$ for pure rotational spectroscopy?
18. What is the effect of isotopic substitution on microwave spectra of linear diatomic molecule?
19. Write a note on Born- Oppenheimer approximation.
20. What is Stark effect? Discuss its applications.
21. What is Raman scattering?
22. Describe the quantum theory of Raman effect.
23. Explain predissociation spectra using a suitable diagram..
24. Write a short note on P,Q and R branches observed in IR spectrum of a diatomic molecule.
25. Note down a principle of ESR spectroscopy.
26. Write down a principle of NMR spectroscopy.
27. Write down a principle of Mossbauer spectroscopy.
28. Discuss the general rules governing the number of lines observed in the ESR spectrum.
29. Discuss the principle of IR spectroscopy in the molecular structure elucidation.
30. What is the significance of zero point energy? Obtain an expression for zero point energy of an anharmonic oscillator.
31. Explain quantum theory of Raman effect.

32. Discuss the theory of pure rotational Raman spectra of linear molecule. Sketch the energy levels and the spectrum arising from transition between them.
33. Write a note on vibrational coarse structure.
34. Write a note on rotational fine structure.
35. How is the dissociation energy of a diatomic molecule determined from vibrational coarse structure in its electronic spectrum?
36. What is force constant? What is its significance? Write the units.
37. Why is CH₄ Raman active?
38. What is Born-Oppenheimer approximation?
39. Explain the variation of intensities of spectral transitions in vibrational- electronic spectra of diatomic molecule.
40. Classify the following molecules based on moment of inertia. H₂O, HCl, C₆H₆, BF₃
41. Define symmetric top and spherical top and give examples of it.
42. What is the equation of rotational constant, B?
43. State and explain rule of mutual exclusion and its converse.
44. What are parallel and perpendicular vibrations? Explain with an example.
45. Explain any two factors which affect the width of spectral lines.
46. Explain classical theory of Raman Effect.
47. Explain photoelectron spectroscopy. Why is high vacuum needed for its study?
48. Discuss rotational fine structure of electronic-vibration transition.
49. Explain the term resolving power and signal to noise ratio.
50. Distinguish between harmonic and anharmonic oscillator with respect to energy, selection rule, and zero point energy.
51. Explain the applications of Mossbauer spectroscopy.
52. Sketch and explain the polarisability ellipsoids for CO₂ molecule.

E) Long answer questions and problems

1. The fundamental vibrational frequency of HCl is 86.63×10^{12} Hz. Calculate zero point energy and force constant for HCl.
2. If band origins at the midpoint of P₁ and R₍₀₎, is at 2143.26 cm^{-1} . This, then is fundamental vibration frequency of CO, if anharmonicity is ignored. First overtone is observed at 4260.04 cm^{-1} . Calculate $\tilde{\omega}$ and x_e .
3. The average spacing between successive rotating lines of CO₂ is 3.826 cm^{-1} . Determine the transition which gives most intense spectral line at 3.
4. The equilibrium vibration frequency of the iodine molecule is 215 cm^{-1} and the anharmonicity constant x_e is 0.003. What is the intensity of the hot band for V=1 to V=2, relative to the fundamental V=0 to V=1, if the temperature is 300K.
5. Show the fluctuations in the dipole moment of carbon dioxide during asymmetric stretching vibrations.
6. Explain various advantages of Fourier transform spectroscopy.
7. Discuss merits and demerits of Raman spectroscopy.
8. Find the value of rotational constant for the molecule ⁷⁹Br¹⁹F if the most intense spectral line at 300K is for the transition J=17 to J=18.
9. The rotational constant for the V=0 state of the molecule is 10 cm^{-1} and V=1 state is 9.5 cm^{-1} . Estimate the rotational constant in the state V=2.

10. How does IR spectroscopy differ from Raman spectroscopy?
11. Pure rotational Raman spectra of linear molecule exhibit first line at $6B \text{ cm}^{-1}$ but remaining at $4B \text{ cm}^{-1}$. Explain.
12. Obtain the expression for moment of inertia for rigid diatomic molecule.
13. The rotational constant for $^{79}\text{Br}^{19}\text{F}$ is 0.35717 cm^{-1} . What is the value of J for which the most intense line will be seen at 300K ?
14. How is the dissociation energy of a diatomic molecule determined from vibrational coarse structure in its electronic spectrum?
15. Calculate the force constant for HCl molecule, as it shows absorption band at 2890 cm^{-1}
[Given: Atomic weight: Cl = 35.5, H = 1.008]
16. What is the effect of breakdown of Born-Oppenheimer approximation on P and R branches of the IR spectrum of a diatomic molecule?
17. The first line in the rotational spectrum of $^{12}\text{C}^{16}\text{O}$ molecule is 3.84235 cm^{-1} . Find out the bond length of the molecule.
18. The Fundamental vibrational frequency of $^1\text{H}^{35}\text{Cl}$ molecule is $86.63 \times 10^{12} \text{ Hz}$. Calculate the zero point energy and force constant of HCl.
19. Explain the factors influencing width and intensity of spectral lines.
20. Explain effect of isotopic substitution on rotational constant B.
21. If band origins at the midpoint of P_1 and $R_{(0)}$, is at 2143.26 cm^{-1} . This, then is fundamental vibration frequency of CO, if anharmonicity is ignored. First overtone is observed at 4260.04 cm^{-1} . Calculate $\tilde{\omega}$ and x_e .
22. The average spacing between successive rotating lines of CO_2 is 3.826 cm^{-1} . Determine the transition which gives most intense spectral line at 300K ?
23. Explain the activity of the following molecules with respect to IR and microwave spectrum. $\text{H}_2, \text{HCl}, \text{CO}_2, \text{CH}_4$ & CH_3Cl
24. What are symmetric and asymmetric vibrations? Explain with the example of H_2O molecule.
- 25.

SECTION-II

A) Multiple choice question

1. In which of the following processes neutrons emitted -
 - e) Inverse beta decay
 - f) Nuclear fission.
 - g) Spontaneous fission
 - h) Nuclear fusion
2. Why neutrons with lower energy should be capable of causing fission?
 - a) For faster reaction processes
 - b) For sustained reaction processes
 - c) For safety purpose
 - d) In order to not waste the nuclear fuel
3. What happens when a neutron is absorbed by a nucleus of an atom of ^{235}U
 - a) Mass number of atom increases
 - b) One electron is let out

- c) ^{236}U isotope is formed
d) Nucleus becomes unstable
4. Who invented nuclear fission?
a) Rutherford
b) Hans Bethe
c) Otto Hahn
d) Marie Curie
5. Atoms of different chemical elements that have the same number of nucleons are called as -
a) isobars
b) isotones
c) isotopes
d) isomers
6. Most of the energy released in fission process is in the form of -
a) Kinetic energy
b) Thermal energy
c) Light energy
d) Heat energy
7. Combining of two light nuclei of low mass to produce a heavy nucleus is called -
a) Nuclear fusion
b) Nuclear fission
c) Spontaneous fission
d) Double beta
8. What type of reaction take place in sun?
a) Nuclear fusion
b) Nuclear fission
c) Spontaneous fission
d) Double beta decay
9. Fusion reactions are called
a) Thermonuclear b) thermoduric c) thermo uric d) compound reactions
10. How is tritium made from sea water?
a) By bombarding lithium
b) By bonding with carbon
c) By bombarding beryllium
d) By reacting with oxygen
11. Which nuclear fuel is usually used in thermal nuclear reactor ton create fission?
a. ^{235}U b) ^{236}U c) ^{234}U d) ^{237}U
12. $^{232}\text{Th}_{90}$ is fertile isotope produced by fission-
a. True b) False

B) One sentence answer

1. Write a definition of natural radioactivity?
2. What is unit of radioactivity?
3. What are the moderators and coolant used in nuclear reactors.

4. Write down different units of radioactivity.
5. Write down four factor formula.
6. Define isobar and isotope.
7. Write down the definition of nuclear fission.
8. Write down principle of G. M. counter.
9. Define "breeder".
10. Write down equation of Decay constant and enlist the terms involved into it.
11. Define the term fission energy.
12. Define the terms fission and fusion.
13. Give one example of beta decay kinetics.
14. Define projectile and ejectile.
15. What is mean by enrichment factor?
16. Define the term 'Dose'.
17. Define the term 'Curie'.

C) Short notes

1. Write a short note on breeder reactors.
2. Write a short note on G.M. counter
3. Write a short note on the classification of reactors.
4. Write in short physico - chemical applications of radioactivity
5. Write a note on neutron activation analysis
6. Write down radiometric titrations.
7. Write a note on isotope separation.
8. Write a note on isotope dilution analysis.
9. Write a short note on radiation dosimetry.
10. Write a short note on radiolysis of water.

D) Short answer question.

1. Write the nuclear reactions involving natural and artificial synthesis of ^3H .
2. Half-life of $\text{Rn} = 3.8$ days, after how many days will $1/20^{\text{th}}$ of Rn sample be left over?
3. Define isotope and isobars.
4. Write down construction and working of GM counter.
5. What are breeder reactors? Explain.
6. Explain the preparation of radiotracer – ^{14}C .
7. Write the four factor formula? Explain the significance of each term involving in it.
8. What are the units of radioactivity? Give the relationship between them.
9. Discuss the principle involving in isotope dilution analysis.
10. What are the primary radiolytic products (prp) of water radiolysis?
11. Write the four factor formula? Explain the significance of each term involving in it.
12. What is separation factor? Explain the electromagnetic method for separation of isotope.
13. Write a note on Fricke dosimeter.
14. Explain three phases in India's nuclear energy programme.
15. What is reproduction factor? Derive Fermi's four factor formula.
16. Explain the principle of isotope dilution analysis.
17. Activity of 1g Ra-226 is found to be 1Ci. How much of it will remain after four half- lives?
18. Define isotope and isobars.
19. Define radioactivity. Write down difference between natural radioactivity and artificial radioactivity.

20. Write down reactions involved in the preparation of radioisotopes ^{35}S and ^{32}P .

E) Long answer questions and problems

1. The activity of a substance drops to $1/32$ of its initial value in ; 1) 7.5 h and 2) 64.45 min. Find its half-life period in two cases.
2. Give an account of nuclear waste management.
3. Discuss the four factor formula used in reactor technology.
4. Give the classification of nuclear reactor.
5. Describe the different types of radioactive decay processes. Give example one example of each.
6. Explain separation of isotopes by the gaseous diffusion method.
7. Give the typical nuclear reactions involving synthesis of ^{32}P and ^{127}I .
8. Explain the nuclear reactions involving natural and artificial synthesis of tritium.
9. Explain the terms – a) Stopping power of medium, b) resolving time of G.M. counter.
10. Explain the preparation of radiotracers – a) ^{22}Na , b) ^{35}S in detail.
11. Discuss the principle of neutron activation analysis (NAA). Explain any two applications of it.
12. Radioisotope can be used to determine diffusion coefficients of the diffusing Species, Explain.
13. Calculate the mass and molecular absorption coefficient for chloroform and

Sodium iodate,

Given; $e \mu = 0.211 \text{ b}$, Z of $\text{Na}=11$, $\text{I} = 53$, $\text{O} = 8$, $\text{C} = 6$, $\text{H} = 1$, $\text{Cl} = 17$.

A of $\text{Na} = 23$, $\text{I} = 127$, $\text{O} = 16$, $\text{C} = 12$, $\text{H} = 1$, $\text{Cl} = 35.5$

14. Note down the types of nuclear reactors based on moderator materials and explain in detail.
15. 0.1 gm. of Mn sample was irradiated with a neutron flux of $1077 \text{ neutron cm}^{-2}\text{s}^{-1}$ for 30 min. What will be its activity at the end of irradiation, if isotopic abundance is 100%, neutron absorption coefficient is 13.3 b and half-life of ^{56}Mn is 2.58 hour?
16. Write down industrial applications-radiation gauging, friction and wear out.