Molecular Spectroscopy MCQs (B.Sc. Level)

General Concepts

1. Which region of the electromagnetic spectrum has the highest energy per photon?
(a) Microwave
(b) Infrared
(c) UV-Visible
(d) Gamma rays
Solution: (d) Gamma rays (Energy is inversely proportional to wavelength, $E = hc/\lambda$. Gamma rays have the shortest wavelength.)

2. The Born-Oppenheimer approximation assumes that...
(a) Electronic and nuclear motions are completely independent.
(b) The nucleus is stationary, as it is much heavier than the electrons.
(c) The total energy of a molecule is the sum of its electronic, vibrational, and rotational energies.
(d) All of the above.
Solution: (b) The nucleus is stationary, as it is much heavier than the electrons. (This allows for the separation of electronic and nuclear motion, leading to (c), but (b) is the core assumption.)

3. The correct order of decreasing energy for molecular transitions is:
(a) Rotational > Vibrational > Electronic
(b) Electronic > Vibrational > Rotational
(c) Vibrational > Electronic > Rotational
(d) Electronic > Rotational > Vibrational
Solution: (b) Electronic > Vibrational > Rotational

Microwave (Rotational) Spectroscopy

4. Microwave spectroscopy is also known as:
(a) Vibrational Spectroscopy
(b) Rotational Spectroscopy
(c) Electronic Spectroscopy
(d) Raman Spectroscopy
Solution: (b) Rotational Spectroscopy (It probes the transitions between quantized rotational energy levels.)

5. Which of the following molecules will show a rotational spectrum?
(a) H_2
(b) Cl_2
(c) HCl
(d) CO_2
Solution: (c) HCl (A molecule must possess a permanent dipole moment to be microwave active.)

6. For a rigid diatomic rotor, the rotational energy levels are given by $E_J = BJ(J+1)$. The selection rule for rotational transitions is:
(a) $\Delta J = 0$
(b) $\Delta J = \pm 1$
(c) $\Delta J = \pm 2$
(d) $\Delta J = 0, \pm 1$
Solution: (b) $\Delta J = \pm 1$

7. In rotational spectroscopy, the separation between adjacent spectral lines for a diatomic molecule is:
(a) B
(b) $2B$
(c) $4B$
(d) $B/2$
Solution: (b) $2B$ (The lines appear at $2B$, $4B$, $6B$, etc., so the separation is $2B$.)

8. The rotational constant B is inversely proportional to:
(a) The reduced mass (μ)
(b) The bond length (r)
(c) The moment of inertia (I)
(d) The rotational quantum number (J)
Solution: (c) The moment of inertia (I) ($B = h / (8\pi^2cI)$)

Infrared (Vibrational) Spectroscopy

9. The region of the electromagnetic spectrum used in Infrared spectroscopy is:
(a) 10-100 cm^{-1}
(b) 400-4000 cm^{-1}

(c) 10,000-25,000 cm^{-1}
(d) 100-200 nm
Solution: (b) 400-4000 cm^{-1} (This is the mid-IR region, most commonly used for vibrational spectroscopy.)

10. The fundamental requirement for a molecule to be IR active is:
(a) It must have a permanent dipole moment.
(b) It must have a change in dipole moment during its vibration.
(c) It must be paramagnetic.
(d) It must be a linear molecule.
Solution: (b) It must have a change in dipole moment during its vibration.

11. Which of the following molecules is IR inactive for its symmetric stretch?
(a) HCl
(b) H_2O
(c) CO_2
(d) NH_3
Solution: (c) CO_2 (During the symmetric stretch $O \leftarrow C \rightarrow O$, the dipoles cancel, and there is no net change in dipole moment.)

12. The vibrational frequency of a diatomic molecule is described by Hooke's Law. The frequency is proportional to:
(a) $(k/\mu)^{1/2}$
(b) $(\mu/k)^{1/2}$
(c) k/μ
(d) μ/k
Solution: (a) $(k/\mu)^{1/2}$ (Where k is the force constant and μ is the reduced mass.)

13. The "fingerprint region" in an IR spectrum is typically:
(a) 4000 - 1500 cm^{-1}
(b) 1500 - 500 cm^{-1}
(c) 3000 - 2000 cm^{-1}
(d) Below 500 cm^{-1}
Solution: (b) 1500 - 500 cm^{-1} (This region contains complex bending vibrations unique to the molecule.)

14. A strong, broad absorption peak around 3300 cm^{-1} in an IR spectrum is characteristic of:
(a) $C=O$ stretch
(b) $O-H$ stretch (alcohol)
(c) $C-H$ stretch (alkane)
(d) $N-H$ stretch (amine)
Solution: (b) $O-H$ **stretch (alcohol)** (The broadness is due to hydrogen bonding.)

15. For a non-linear molecule with N atoms, the number of vibrational modes is:
(a) $3N - 5$
(b) $3N - 6$
(c) $3N$
(d) $3N - 4$
Solution: (b) $3N - 6$ (A linear molecule has $3N - 5$ modes.)

Raman Spectroscopy

16. Raman spectroscopy is based on the:
(a) Absorption of light
(b) Emission of light
(c) Scattering of light
(d) Diffraction of light
Solution: (c) Scattering of light

17. The lines in a Raman spectrum with a lower frequency (longer wavelength) than the incident light are called:
(a) Rayleigh lines
(b) Stokes lines
(c) Anti-Stokes lines
(d) Resonance lines
Solution: (b) Stokes lines (The molecule gains energy from the photon, which is scattered with less energy.)

18. The fundamental requirement for a molecule to be Raman active is:
(a) A permanent dipole moment
(b) A change in dipole moment during vibration
(c) A change in polarizability during vibration
(d) The presence of unpaired electrons
Solution: (c) A change in polarizability during vibration

19. According to the mutual exclusion principle, for

a centrosymmetric molecule (like CO_2):
(a) Vibrations active in IR are also active in Raman.
(b) Vibrations active in IR are inactive in Raman, and vice versa.
(c) All vibrations are inactive in both.
(d) All vibrations are active in both.
Solution: (b) Vibrations active in IR are inactive in Raman, and vice versa.

20. In Raman spectroscopy, which lines are more intense at room temperature?
(a) Stokes lines
(b) Anti-Stokes lines
(c) Rayleigh lines
(d) Both Stokes and Anti-Stokes are equally intense.
Solution: (a) Stokes lines (They originate from the ground vibrational state, which is more populated than excited states at room temperature.)

UV-Visible (Electronic) Spectroscopy

21. UV-Visible spectroscopy involves transitions of:
(a) Rotational energy levels
(b) Vibrational energy levels
(c) Electronic energy levels
(d) Nuclear spin states
Solution: (c) Electronic energy levels
(Specifically, transitions of valence electrons.)

22. Which electronic transition requires the highest energy?
(a) $\sigma \to \sigma^*$
(b) $n \to \sigma^*$
(c) $\pi \to \pi^*$
(d) $n \to \pi^*$
Solution: (a) $\sigma \to \sigma^*$ (These involve strongly bonded sigma electrons and are usually found in the far-UV.)

23. The Beer-Lambert Law is given by $A = \epsilon cl$. What does ϵ (epsilon) represent?
(a) Absorbance
(b) Path length
(c) Concentration
(d) Molar absorptivity (or extinction coefficient)
Solution: (d) Molar absorptivity (or extinction coefficient)

24. A group that imparts color to a molecule is called a:
(a) Chromophore
(b) Auxochrome
(c) Isotope
(d) Homologue
Solution: (a) Chromophore (e.g., $C=C$, $C=O$, $N=N$)

25. A shift of an absorption band to a longer wavelength (lower energy) is known as:
(a) Hypsochromic shift (blue shift)
(b) Bathochromic shift (red shift)
(c) Hyperchromic effect
(d) Hypochromic effect
Solution: (b) Bathochromic shift (red shift)

26. An auxochrome is a group that:
(a) Absorbs UV light itself.
(b) Is a saturated group that, when attached to a chromophore, shifts the absorption to a longer wavelength.
(c) Decreases the color intensity.
(d) Is responsible for fluorescence.
Solution: (b) Is a saturated group that, when attached to a chromophore, shifts the absorption to a longer wavelength. (e.g., $-OH$, $-NH_2$)

27. An increase in absorption intensity (ϵ_{max}) is known as a:
(a) Hyperchromic effect
(b) Hypochromic effect
(c) Bathochromic shift
(d) Hypsochromic shift
Solution: (a) Hyperchromic effect

NMR (Nuclear Magnetic Resonance) Spectroscopy

28. NMR spectroscopy is based on the absorption of radiofrequency waves by:
(a) Electrons in a magnetic field
(b) Atomic nuclei in a magnetic field
(c) Vibrating molecules
(d) Rotating molecules
Solution: (b) Atomic nuclei in a magnetic field

(Specifically, nuclei with a non-zero spin, like ^1H or ^{13}C.)

29. The standard reference compound used in ^1H NMR spectroscopy is:
(a) Carbon tetrachloride (CCl_4)
(b) Tetramethylsilane (TMS)
(c) Chloroform ($CDCl_3$)
(d) Benzene (C_6H_6)
Solution: (b) Tetramethylsilane (TMS) (It is chemically inert, and its 12 equivalent protons give a single, sharp signal at $\delta = 0$.)

30. The phenomenon of "chemical shift" in NMR refers to:
(a) The splitting of a signal into multiple peaks.
(b) The position of a signal in the spectrum, relative to the reference.
(c) The intensity of the signal.
(d) The relaxation time of the nucleus.
Solution: (b) The position of a signal in the spectrum, relative to the reference. (It's caused by the shielding or deshielding of the nucleus by surrounding electrons.)

31. Protons that are in a more electron-dense environment are said to be:
(a) Shielded, and absorb at a higher δ value (downfield).
(b) Shielded, and absorb at a lower δ value (upfield).
(c) Deshielded, and absorb at a higher δ value (downfield).
(d) Deshielded, and absorb at a lower δ value (upfield).
Solution: (b) Shielded, and absorb at a lower δ value (upfield). (They feel a weaker effective magnetic field.)

32. The splitting of an NMR signal into a multiplet is caused by:
(a) Chemical shift
(b) Spin-spin coupling
(c) Nuclear shielding
(d) The magnetic field strength
Solution: (b) Spin-spin coupling (The interaction of spins of adjacent, non-equivalent nuclei.)

33. According to the ($n+1$) rule, a proton with 'n' adjacent, equivalent protons will have its signal split into:
(a) n peaks
(b) $n+1$ peaks
(c) $2n$ peaks
(d) $n-1$ peaks
Solution: (b) $n+1$ peaks

34. How many signals would you expect in the ^1H NMR spectrum of ethanol (CH_3CH_2OH)?
(a) 1
(b) 2
(c) 3
(d) 4
Solution: (c) 3 (There are three sets of non-equivalent protons: the CH_3 group, the CH_2 group, and the OH group.)

35. What splitting pattern would be observed for the CH_2 group in ethanol (CH_3CH_2OH) (assuming coupling to OH is not observed)?
(a) Singlet
(b) Doublet
(c) Triplet
(d) Quartet
Solution: (d) Quartet (The CH_2 group is adjacent to the CH_3 group, which has $n=3$ protons. $n+1 = 3+1 = 4$.)

36. The area under an NMR signal (integration) is proportional to:
(a) The number of protons giving rise to the signal.
(b) The number of adjacent protons.
(c) The chemical shift.
(d) The coupling constant (J).
Solution: (a) The number of protons giving rise to the signal.

37. Which of the following nuclei is not NMR active?
(a) ^1H
(b) ^{13}C
(c) ^{12}C
(d) ^{19}F
Solution: (c) ^{12}C (It has an even mass number and even atomic number, so its nuclear spin $I=0$.)

38. The ^1H NMR spectrum of benzene (C_6H_6) shows:
(a) A single peak (singlet)
(b) A doublet
(c) A triplet
(d) Six different peaks
Solution: (a) A single peak (singlet) (All six protons are chemically and magnetically equivalent due to symmetry and ring current.)

39. In ^{13}C NMR, a "proton-decoupled" spectrum means:
(a) All carbon signals are removed.
(b) All proton signals are removed.
(c) All $^{13}C-^1H$ coupling is removed, making each carbon signal a singlet.
(d) All $^{13}C-^{13}C$ coupling is removed.
Solution: (c) All $^{13}C-^1H$ **coupling is removed, making each carbon signal a singlet.**

40. How many signals would be present in the proton-decoupled ^{13}C NMR spectrum of toluene ($C_6H_5CH_3$)?
(a) 2
(b) 4
(c) 5
(d) 7
Solution: (c) 5 (Due to symmetry, there are 5 unique carbons: the CH_3 carbon; the C attached to the CH_3; the ortho carbons (2); the meta carbons (2); and the para carbon (1).)