

# Spectroscopy (Rotational, Vibrational, Raman, electronic) [ \* denotes for advance studies ]

(Question lists for University examination)

1. What is spectroscopy?
2. Regions of spectrum & units.
3. Derive the expressions for rotational energy of a diatomic molecule considering it to be a rigid rotator.
4. What is selection rule?
5. "Rotational lines are equispaced"  $\rightarrow$  explain.
- \* 6. Rotational lines for non-rigid rotator are not equispaced  $\rightarrow$  clarify.
7. Derive an expression for vibrational energy of a diatomic molecule considering Harmonic vibration.
- \* 8. In vibrational spectroscopy only one absorption line is observed. Justify.
9. Why does the vibration of a diatomic molecule is Anharmonic in nature?
10. Write down an expression for vibrational energy for a diatomic molecule considering anharmonic vibration.
11. What is the essential Condition for a molecule to give vibrational spectra?
12. Calculate the number of vibrational modes of  $H_2O$ . Give a pictorial representation of normal modes.
13. What is vibration-rotation spectrum? In which region of the electromagnetic radiation does it appear?
14. Discuss the breakdown of Born-Oppenheimer approximation.
15. What is electronic spectra of diatomic molecule?
- \* 16. In case of atoms vibrational & rotational spectra do not take place  $\rightarrow$  Justify.
17. What is Raman Scattering? How does it differ from Rayleigh Scattering?
18. What is the essential Condition for a molecule to be Raman active?



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19. Discuss the rotational, Raman & vibrational Raman spectra.
20. Discuss the polarization of Raman lines.
- \* 21. What is CARS & RRS? What are their applications?
- \* 22. What is totally symmetric representation?
- \* 23. What is polarised light?
- \* 24. What is LASER? Discuss the use of LASER in Raman Spectroscopy? Discuss the types of LASER (without derivations)
- \* 25. Discuss CO<sub>2</sub> LASER? Why N<sub>2</sub> is mixed in this case?
- \* 26. What is Signal to noise ratio (S/N)?
27. Discuss Frank-Condon principle?
28. What is Overtone bands?
29. Discuss about Fermi resonance, Hot band, Fundamental v.v.t bands, combination band and Coupled vibration.
- \* 30. What is Vibronic Coupling?
31. What is mutual exclusion principles?
- \* 32. What are PR, PQR bands?
33. Discuss the selection rules for polyatomic molecules in Rotational, Vibrational and Roto-vibrational spectra.
- \* 34. What is Femto-second LASER?
35. Which of the following molecules will show a pure rotational spectrum?  
HCl, CO, H<sub>2</sub>, CH<sub>3</sub>Cl, H<sub>2</sub> (liq.), NH<sub>3</sub>, NH<sub>4</sub>Cl (s)
36. Which of the following molecules will show vibrational spectrum?  
CH<sub>3</sub>Cl, HCl, CO, H<sub>2</sub>, H<sub>2</sub>O, NH<sub>3</sub>, NH<sub>4</sub>Cl, C<sub>2</sub>H<sub>6</sub>, C<sub>6</sub>H<sub>6</sub>, CCl<sub>4</sub>, CO<sub>2</sub>
37. Which of the following molecules will show a rotational Raman spectrum?  
SF<sub>6</sub>, C<sub>2</sub>H<sub>6</sub>, NH<sub>3</sub>, H<sub>2</sub>O, CH<sub>3</sub>Cl, CH<sub>4</sub>, CO, HCl, H<sub>2</sub>
38. Which of the following molecules will show a vibrational Raman spectrum?  
H<sub>2</sub>, HCl, CO, CH<sub>4</sub>, CH<sub>3</sub>Cl, H<sub>2</sub>O, NH<sub>3</sub>, C<sub>2</sub>H<sub>6</sub>, SF<sub>6</sub>



39. What is Stokes and Anti Stokes lines?
  40. What is Spherical top and Symmetric top molecules?
  41. "All IR active bands are Raman active" — Criticise the statement.
  - \*42. What is Line spectra, Band spectra, Continuous spectra?
  43. Is there any difference between Continuous spectra and band spectra?
  44. Kinetic energy is Quantised — Criticise the statement. (Think: moving in space is not quantised)
  45. Kinetic energy ~~gives~~ ~~Continuous~~ ~~Continuous~~ results Continuum spectra — Justify or Criticise.
  - \*46. What is ~~Convergence~~ Convergence limit for Balmer series?
  47. What is Raman Scattering and Fluorescence scattering?
  - \*48. Why we <sup>generally</sup> get more ~~than~~ lines in IR spectra despite of having limited theoretical fundamental ~~and~~ modes?
  49. Discuss the use of Far-IR spectra for the determination of structure of a molecule.
  50. What is degrees of freedom? How many normal modes of vibration can be expected in the following molecules?
- $\text{H}_2\text{O}$  ,  $\text{N}_2$  ,  $\text{NCS}$  ,  $\text{SO}_2$  ,  $\text{N}_2\text{F}_2$  (cis)  
 $\text{CO}_2$  ;  $\text{H}_2\text{O}_2$  ,  $\text{CNO}$  ,  $\text{HCN}$  ,  $\text{N}_2\text{F}_2$  (trans)  
 $\text{CH}_4$  ,  $\text{CH}_3\text{Cl}$  ,  $\text{CHCl}_3$  ,  $\text{NH}_3$  ,  $\text{BF}_3$  ,  $\text{SF}_6$
51. What is Compound doublet?
  52. What is Singlet State? What is Triplet State?
  53. Singlet Oxygen are reactive — Explain.
  54. ~~Discuss~~ Discuss the spectrum of Lithium and other hydrogen like species.
  55. Discuss the spectrum of Helium and alkaline earth metal.
  56. What is dissociation energy?