

PHY4C12:ATOMIC AND MOLECULAR SPECTROSCOPY

A Part

1. Explain the concept of space quantisation.
2. Explain singlet and triplet states with examples.
3. The magnetic moment μ of an atom never points in the z direction. Explain.
4. The magnetic moment μ of an atom never points in the z direction. Explain.
5. Give two important features of vector atom model.
6. Write a note on L-S coupling scheme.
7. Explain the concept of space quantization.
8. What is Larmor precessional frequency?
9. Explain the L-S coupling scheme for the addition of angular momenta.
10. Distinguish between singlet and triplet states with examples.
11. Write a note on LS coupling.
12. Briefly explain the important features of vector atom model.
13. Distinguish between singlet and triplet states with examples.
14. Write a note on interaction energies of L S coupling and j-j coupling schemes.
15. Discuss the concept of spectral terms and their notations in jj coupling with a suitable example.
16. Write a note on j-j coupling scheme.
17. Write a note on jj coupling.
18. Explain J-J coupling scheme.
19. Distinguish between Zeeman effect and Paschen Back effect
20. What is Zeeman splitting of spectral line?
21. Write a note on the intensity of Zeeman lines.
22. Give the classical theory of normal Zeeman effect.
23. What is Zeeman effect? Distinguish between normal and anomalous Zeeman effect.
24. Distinguish between Paschen-Back, normal and anomalous Zeeman effect.
25. What is the difference between Zeeman effect and Stark effect?
26. Explain Stark Effect.
27. Write a note on Paschen Back Effect
28. Write a note on weak field Stark effect in hydrogen atom.
29. Explain complete Paschen- Back effect

30. Explain the effect of anharmonicity on the vibrational spectra of diatomic molecules.
31. Explain the effect of centrifugal distortion on the moment of inertia and energy of a diatomic molecule.
32. Elucidate the salient microwave spectral features of symmetric top molecule.
33. Write a note on the intensity of the spectral lines of rotational spectra.
34. Outline the procedure to obtain moment of inertia and inter atomic distance using the technique of microwave spectroscopy.
35. Compare the rotational energy levels of a rigid prolate and rigid oblate symmetric top molecules and schematically represent the transitions.
36. In the rotational spectra of a diatomic molecule the separation between adjacent lines is found to decrease with increase in rotational quantum number J . Give reason.
37. Explain why homonuclear diatomic molecules are microwave inactive.
38. What is centrifugal distortion? Describe the effect of centrifugal distortion on the moment of inertia and energy of diatomic molecule.
39. What are hot bands? Why are they called so?
40. Obtain an expression for rotational energy levels of a non-rigid diatomic molecule and schematically represent it.
41. Write a note on intensity of rotational spectral lines. Write the equation for the most intense line?
42. Give a brief account of the rotational energy levels and spectra of rigid prolate symmetric top molecule.
43. Explain the spectrum of a non-rigid rotator.
44. In terms of the principal moments of inertia, how are molecules classified?
45. Explain the isotope effect in pure rotational spectra.
46. What are the salient features of rotational spectra?
47. List the differences between atomic and molecular spectroscopy.
48. Explain the rotational spectrum of CH_3Cl molecule.
49. Homonuclear diatomic molecules do not show vibrational spectra. Why?
50. What are the informations that can be derived from the rotational spectrum of a molecule?
51. Which of the following molecules will show a microwave rotational spectrum: H_2 , HCl , CH_4 , CH_3Cl ? Why?
52. What is the role of Stark modulator in a microwave spectrometer?
53. What are hot bands? Why are they called so?
54. Homonuclear diatomic molecules do not show vibrational spectra. Why?
55. Discuss the effect of breakdown of Born – Oppenheimer approximation in molecular spectra.
56. What is Born Oppenheimer approximation? Based on this approximation, what are the salient features of rotation vibration spectra of diatomic vibrating rotor.

57. What are hot bands? Why are they called so?
58. Explain the terms overtones and hot bands.
59. What is Born Oppenheimer approximation? What is the effect of break down of this approximation?
60. Alternate lines of P and R branches in the spectrum of acetylene (C_2H_2) are less intense. Why?
61. Explain the effect of anharmonicity on the vibrational spectra of a diatomic molecule.
62. What are hot bands?
63. Write a note on normal modes of vibrations of CO_2 molecule.
64. What is the principle of FTIR spectrometer?
65. What is the advantage of fourier transform IR spectroscopy over conventional IR technique?
66. Write a note on FTIR spectroscopy.
67. Write a note on modes of vibrations of polyatomic molecules with suitable examples.
68. Draw the schematic diagram of IR spectrometer.
69. Give a brief account of the normal modes of vibrations of carbon dioxide molecule.
70. Hydrogen molecule gives no microwave or infrared spectra whereas they give a rotational Raman spectrum. Why?
71. In linear molecules, the Raman shift of the first Stokes/anti Stokes line from the exciting one is $6B$ whereas it is $4B$ in symmetric top molecules. Why?
72. Discuss the rotational Raman spectra of symmetric top molecules.
73. What are stokes and anti-stoke lines?
74. The rotational Raman spectrum of CH_3Cl molecule shows an alternation in intensity. Why?
75. Write the expression for the ratio of the intensity between the Stokes and anti Stokes lines.
76. Which is more intense in Raman lines - stokes lines or antistokes line? Why?
77. Discuss the rotational Raman spectra of linear molecules.
78. Compare the IR and Raman activities of the normal modes of vibration of carbon dioxide and water molecules.
79. Explain the difference between Raman spectra and IR spectra.
80. Comment on the vibrational Raman spectra of linear molecules.
81. Explain why homonuclear diatomic molecules give no microwave or infrared spectra but give a rotational Raman spectrum.
82. Name the fundamental modes of vibrations of CO_2 molecule and with appropriate reasoning, predict its IR and Raman active modes.
83. Explain the conditions for a vibration to be Raman active taking the normal vibrations of CO_2 molecule as example.

84. Write the applications of Raman Effect.
85. Illustrate mutual exclusion principle with an example.
86. In H_2 molecule the separation between adjacent rotational Raman lines is $4B$ whereas in O_2 it is $8B$. Why?
87. Illustrate mutual exclusion principle.
88. What are the basic requirements for observing inverse Raman scattering?
89. Explain non-linear Raman effect.
90. What are the basic requirements for observing hyper-Raman effect?
91. Explain the basic principle of stimulated Raman scattering.
92. Compare Hyper Raman effect and stimulated Raman scattering.
93. Explain with diagrams inverse anti-stokes Raman scattering and inverse stokes Raman scattering.
94. Very intense light sources are needed for the observation of non linear Raman effects. Why?
95. Explain Stimulated Raman Effect.
96. Explain the basic principle of stimulated Raman scattering.
97. Explain hyper Raman effect.
98. What is inverse Raman Effect?
99. Write a note on Déslandre's table.
100. What is a v' progression? Comment on the relative energy of spectral lines in v' progression.
101. Distinguish between ν' and ν'' progression.
102. Explain with diagrams progressions and sequences.
103. State Franck-condon principle.
104. Write a note on Frank – Condon principle.
105. Discuss Frank – Condon principle.
106. What information is generated from the vibrational analysis of electronic spectra ?
107. What all information do we get from the vibrational analysis of electronic spectra?
108. Explain dissociation energy.
109. What is Fortrat parabola? Explain the significance of band head and band origin.
110. Write a note on Fortrat Diagram
111. Distinguish between the dissociation energies D_e and D_0 .
112. Band head of rotational fine structure of electronic- vibration transition of a molecule is at a frequency higher than that of band origin. What does this imply?
113. Explain band head and band origin in the rotational fine structure of electronic vibration spectra.

114. Distinguish between dissociation energies $D_{\{e\}}$ and $D_{\{o\}}$.
115. What is the principle of NMR spectroscopy?
116. What kind of nuclei show NMR spectrum? What is the resonance condition in NMR spectroscopy?
117. What is the frequency range in which NMR spectrum is obtained? How is it related to external magnetic field?
118. C-12 nuclei do not show NMR spectrum where as C-13 nuclei show NMR spectrum. Explain.
119. Compare the MNR spectra of a spin half nucleus with that of a spin 1 nucleus.
120. What is meant by relaxation process? Explain spin- spin relaxation.
121. Distinguish between spin lattice and spin spin relaxation.
122. Explain spin- lattice relaxation process in NMR. Define relaxation time
123. Explain relaxation process in NMR.
124. Draw the NMR spectrum of acetaldehyde (CH_3CHO). What causes the shift in the spectrum?
125. Obtain an expression for the chemical shift in NMR. What is the advantage of using TMS as reference?
126. With a suitable example, explain chemical shift in NMR.
127. What do you mean by spin-spin relaxation?
128. Outline the principle of ESR spectra.
129. Obtain the resonance condition in ESR spectroscopy.
130. Discuss the ESR spectra of Hydrogen atom.
131. ESR spectrum is usually recorded in first derivative mode. Why?
132. What are the different factors contributing to the total hamiltonian of an electron?
133. Explain the hyperfine structure in ESR spectra of an electron coupled to a nucleus of spin $1/2$.
134. Draw the ESR Spectrum of hydrogen atom.
135. Comment on the intensity of spectral lines in the hyperfine structure of the ESR spectrum of an unpaired electron coupled with two equivalent nuclei of spin $1/2$.
136. What do you mean by hyperfine structure in ESR spectroscopy?
137. What is Fermi Contact interaction?
138. Explain the factors responsible for hyperfine structure in ESR spectra.
139. Obtain an expression for the recoil velocity of a nucleus when a gamma ray is emitted.
140. Why do recoil velocity of nucleus is so important in Mossbauer Spectroscopy?
141. Outline the principle of Mossbauer spectroscopy.
142. What makes Mossbauer spectroscopy distinct as compared to other spectroscopic techniques?
143. Discuss recoilless emission and absorption of gamma rays.

144. Discuss the principle behind Mossbauer Spectroscopy.
145. Write a note on isomer shift?
146. What is isomer shift in Mossbauer spectroscopy? Obtain an expression for it.
147. What are the techniques used in Mossbauer spectroscopy to compensate the energy loss due to recoil of the nucleus?
148. What are the applications of Mossbauer spectroscopy?
149. How do recoilless emission and absorption are achieved in Mossbauer spectrometer?
150. Write brief note on (1) Mossbauer sources and (2) absorbers.

B Part

151. What are the main concepts in vector atom model? Discuss in detail the L-S and jj coupling schemes for a two electron system.
152. Illustrate the L-S coupling scheme for a two electron system with an example. Deduce the different interaction energy terms in L-S coupling.
153. Illustrate the jj coupling scheme in a two electron system with an example. Deduce the different interaction energy terms in jj coupling.
154. Derive an expression for Lande splitting factor in a two electron system. Illustrate the theory of anomalous Zeeman effect and obtain an expression for the interaction energy. Compare the spectra produced by singlet and triplet states.
155. Describe the effect of magnetic field on the spectra of atoms. Distinguish between normal and anomalous Zeeman Effect with an example.
156. Discuss in detail, the anomalous Zeeman Effect in a single electron system and obtain the expression for magnetic interaction energy
157. Explain the theory of anomalous Zeeman effect. Illustrate with diagrams of the Zeeman splitting of Sodium Yellow D lines. Comment on the relative intensities of the spectral lines.
158. Explain with theory the Zeeman Effect shown by a two electron system and draw the Zeeman pattern corresponding to a principal series triplet.
159. With necessary theory account for the splitting of atomic spectral lines in the presence of a weak magnetic field.
160. Describe the normal and anomalous Zeeman effect. Explain the Zeeman effect in the spectrum of sodium atom with a diagram.
161. Outline the theory of Paschen Back effect in a two electron system and obtain an expression for the interaction energy. Calculate the energy terms for 3S state and draw the strong field energy levels.
162. Distinguish between Paschen -Back effect and complete Paschen- Back effect. Deduce the interaction energy terms in each of these cases.
163. What is Stark effect? Explain the weak field Stark effect in hydrogen atom.
164. What is Paschen Back effect? With necessary theory discuss the Paschen Back pattern for a $^2P - ^2S$ transition.

165. Discuss in detail the spectrum of non-rigid rotator and obtain the expression for frequencies of the spectral transitions of a symmetric top molecule.
166. Explain with necessary theory the spectral transitions of non-rigid rotator.
167. Discuss the rotational spectra of a rigid diatomic molecule. Obtain an expression for the J value for which the transition intensity is maximum. What happens to the spectrum if the molecule is a non-rigid one?
168. Discuss the rotational spectra of diatomic molecules as a rigid rotator. Draw energy level diagram and show transitions.
169. Discuss, with necessary equations and energy level diagram, the rotational spectra of rigid diatomic molecules. What is the effect of isotope substitution on the spectrum?
170. Discuss with suitable diagram, the theory and working of microwave spectrometer and write a note on information derived from the rotational spectra.
171. Describe the construction and working of microwave spectrometer.
172. Discuss the rotational vibrational spectra of diatomic molecules. What causes the asymmetry in the spectrum?
173. With necessary energy level diagram discuss the rotational fine structure of vibrational band in a diatomic vibrating rotator.
174. With necessary theory, give an account of rotation vibration spectrum of a diatomic molecule. Give reason for the asymmetry of experimental rotation vibration band.
175. Explain how the study of vibrational spectrum of a diatomic molecule enables us to determine the anharmonicity constant and equilibrium frequency of vibration.
176. Explain the theory of rotational - vibrational spectra of diatomic molecules.
177. Explain with a neat diagram, the working of IR double beam spectrophotometer.
178. Describe the instrumentation of IR spectroscopy. Write a note on FTIR spectroscopy. What is the advantage of Fourier transform over the conventional technique?
179. Explain the technique of FTIR spectroscopy. What is its advantage over conventional IR technique?
180. With the help of a schematic diagram, describe the construction, working and advantages of FTIR spectroscopy.
181. Describe normal modes of vibrations of CO_2 and H_2O . Explain the instrumentation of IR spectroscopy.
182. With a block diagram describe the construction and working of Raman Spectrometer
183. Discuss rotational Raman spectrum of linear molecule and symmetric top molecules
184. Give the quantum theory of Raman effect. How rotational energy changes in molecules can be studied using Raman effect?
185. With the help of a schematic diagram, describe the construction and working of a Raman spectrometer.
186. With block diagram, describe the laser Raman spectrometer and outline the advantages of using laser as a Raman source.
187. Write notes on 1. Mutual exclusion principle. 2. Polarised Raman lines and depolarisation ratio. 3. Intensity of stokes and antistokes lines.

188. Discuss in detail, how structure of diatomic and triatomic molecules can be determined by combining Raman and Infra-red spectroscopy.
189. Explain how the structure of XY_2 type and XY_3 type is determined using Raman and Infra-Red spectroscopy.
190. Draw the Block Diagram of Raman Spectrometer and explain the working.
191. What is Deslandre's table? Explain progressions & sequences in electronic spectroscopy of molecules.
192. Explain with necessary theory, how the vibrational analysis of band systems of electronic spectra enables us to determine anharmonicity constant χ_e and equilibrium frequency of vibration ν_e .
193. a) Discuss in detail the rotational fine structure of electronic vibration spectra b) Write a short note on Fortrat Parabolae.
194. Discuss in detail the rotational fine structure of electronic vibrational transitions.
195. Discuss in detail the rotational fine structure of electronic vibrational transitions
196. Discuss in detail, the rotational fine structure of electronic -vibration transitions and mark the P, Q and R branches in the diagram.
197. Discuss in detail the rotational fine structure of electronic vibrational spectra. Obtain equations for frequencies corresponding to $\bar{\nu}_P$, $\bar{\nu}_Q$ and $\bar{\nu}_R$.
198. Explain the principle of NMR spectroscopy and its applications.
199. (1) Explain different relaxation processes for nuclei. (2) Explain chemical shift in NMR spectra with an example.
200. Explain different relaxation processes for nuclei and briefly explain chemical shift in NMR spectra.
201. Deduce Bloch equation and its steady state solutions.
202. Explain the basic principles of NMR spectroscopy. Derive Bloch equations.
203. Explain different relaxation processes for nuclei and derive Bloch equation.
204. Explain different relaxation processes for nuclei and derive Bloch equations
205. Derive Bloch equations.
206. Explain the basic principles of Electron spin resonance spectroscopy. Discuss the hyperfine components in the ESR spectrum of a system having an unpaired electron interacting with (1) a nucleus of spin 1 (2) two non equivalent protons.
207. Explain the basic principles of Electron spin resonance spectroscopy. Discuss the hyperfine components in the ESR spectrum of a system having an unpaired electron interacting with (1) two equivalent protons (2) two non equivalent protons.
208. Explain the principle of ESR technique. Discuss the working of ESR spectrometer with the help of a schematic diagram.
209. Give the basic principles of Mossbauer effect. With the help of a schematic diagram describe the construction and working of Mossbauer spectrometer.
210. Discuss the principle of Mossbauer spectroscopy. Write notes on isomer shift and magnetic hyperfine interaction in Mossbauer spectroscopy.

211. Write notes on isomer shift and magnetic hyperfine interaction in Mossbauer spectroscopy.

C Part

212. Find out the different spectroscopic terms arising from the interaction of two electrons in pd configuration in L-S coupling. Which term will have the lowest energy? Explain.

213. Consider two electrons, one in the 4p and the other in the 4f subshell. Obtain the possible L, S and J values and the term symbols for this two electron system.

214. What is Larmour precession? Obtain expression for Larmour frequency.

215. In an atom, obeying L-S coupling, the components of a normal triplet state have separations 20 and 40 cm^{-1} between adjacent components. There is a higher state for which the separations are 22 and 33 cm^{-1} respectively. Determine the terms for the two states and show with the help of an energy level diagram the allowed transitions and the pattern of the spectrum.

216. Explain Hund's rule with an example.

217. Obtain Lande g factor for the level 3D_3 and 3P_1 . Obtain angle between orbital and spin angular momentum vectors.

218. Evaluate the different spectroscopic terms arising due to (1) an electron in p orbital and another electron in f orbital and (2) an electron in p orbital and another electron in d orbital in L-S coupling.

219. Find the possible term values for two electrons in the configuration p.d and d.d under L-S coupling.

220. Consider a hydrogen atom in $D_{3/2}$ state. (i) Find the possible values of J_z (ii) What are different orientations of J vector in space?

221. Consider a hydrogen atom in the $D_{3/2}$ state. (i) Find the possible values of J_z (ii) What are the different orientations of the J-vector, in space.

222. Obtain the terms obtained from the coupling of (1) one p-electron and one d-electron and (2) one s electron and one f electron in L-S coupling.

223. Evaluate the different spectroscopic terms arising due to an electron in p orbital and another electron in f orbital in j-j coupling. How are the terms represented?

224. Evaluate the different spectroscopic terms arising due to the interaction of an electron in p orbital and another electron in d orbital in j-j coupling. How are the terms represented?

225. The calcium line of wavelength 4226.73 Å exhibits normal Zeeman splitting when placed in uniform magnetic field of 4 weber /meter². Calculate the positions of three components of normal Zeeman pattern in cm^{-1} and separation between them.

226. Derive the expression for Lande's g factor

227. Explain the classical theory of Zeeman Effect and obtain the expression for the Zeeman shift.

228. Draw the normal Zeeman Pattern for 1F_3 to 1D_2 transition.

229. Calculate the splitting factors for the 2P and 2S levels and draw the anomalous zeeman pattern for the sodium D_1 and D_2 lines.

230. Calculate the interaction energy terms in a strong magnetic field for a two electron system in sp configuration.

231. Deduce the interaction energy terms in complete Paschen-Back effect in a two electron system
232. Rotational and centrifugal distortion constants of HCl molecules are 10.593cm^{-1} and $5.3 \times 10^{-4}\text{cm}^{-1}$ respectively. Estimate the vibrational frequency and force constant of the molecule.
233. Rotational and centrifugal distortion constants of HCl molecule are 10.593cm^{-1} and $5.3 \times 10^{-4}\text{cm}^{-1}$ respectively. Estimate the vibrational frequency and force constant of the molecule.
234. What is the change in the rotational constant B when hydrogen is replaced by deuterium in the hydrogen molecule?
235. What is the average speed of rotation of HCl molecule if it is in the $J = 1$ state? The internuclear distance of HCl is 0.1274nm . Given mass of hydrogen and chlorine atoms are $1.673 \times 10^{-27}\text{kg}$ and $58.06 \times 10^{-27}\text{kg}$ respectively.
236. Which of the following molecules have a microwave spectrum? Explain the reason. (a) O_2 (b) HCl (c) IF (d) F_2
237. The observed rotational spectrum of HF shows the $J = 0 \rightarrow J = 1$ absorption at 41.11cm^{-1} , the spacing between adjacent absorptions is 40.08cm^{-1} around $J = 5 \rightarrow J = 6$ transition and only 37.81cm^{-1} around $J = 10 \rightarrow J = 11$ transition. Calculate B values and I values from these three given data. What explanation can you give for this variation?
238. If the wavenumber of the $J = 2$ to 3 rotational transition of $^1\text{H}^{35}\text{Cl}$ considered as a rigid rotor is 63.56cm^{-1} . Calculate the moment of inertia of the molecule and the bond length.
239. How many revolutions per second does a CO molecule make when $J = 4$. The rotational constant of CO molecule is 1.9313cm^{-1}
240. The average line spacing between successive rotational lines of CO molecule is 3.8626cm^{-1} . Determine the transition which give the most intense line at room temperature.
241. Two consecutive lines of the rotational spectrum of HCl molecule are observed at 211.86cm^{-1} and 233.046cm^{-1} . Calculate the values of rotational constant B, distortion constant D and rotational quantum number J of these transitions. μ of HCl = $1.6261 \times 10^{-27}\text{kg}$ and the force constant of the bond = 517.8Nm^{-1} .
242. Three consecutive lines in the rotational spectrum of a diatomic molecule are observed at 84.544 , 101.355 and 118.112cm^{-1} . Assign these lines to their appropriate $J \rightarrow J'$ transitions and deduce values of B and D. Hence evaluate the approximate vibrational frequency of the molecule.
243. The first line in the rotation spectrum of carbon monoxide has a frequency of 3.8424cm^{-1} . Calculate the rotational constant and hence the C-O bond length in carbon monoxide. Avagadro number is $6.022 \times 10^{23}/\text{mol}$.
244. The rotational constant for CO is 1.9314cm^{-1} and 1.6116cm^{-1} in the ground and first excited vibrational states, respectively. By how much does the internuclear distance change as a result of this transition?
245. The spacing of a series of lines in the micro wave spectrum of AlH is constant at 12.604cm^{-1} . Calculate the moment of Inertia and the inter nuclear distance of the AlH molecule. What are the energy of rotation and rate of rotation when $J = 15$? Mass of Al is 26.9815u .
246. The separation between the lines in the rotational spectrum of HCl molecule was found to be 20.92cm^{-1} . Find its bond length and also find the most intense line at 300K . Mass of H = 1.008u and that of Cl = 35.46u .

247. Calculate the rotational constant and bond length of CO. Given, rotational band line spacing 3.86 cm^{-1} .
248. Derive expression for the frequencies of the Stark components of the $J = 1 \rightarrow J = 2$ transitions of a linear molecule.
249. Draw the energy levels and spectral lines of a diatomic vibrating rotator.
250. The fundamental and first overtone transition of $^{14}\text{N}^{16}\text{O}$ are centred at 1876.06 cm^{-1} and 3724.20 cm^{-1} respectively. Evaluate the equilibrium vibration frequency, the anharmonicity constant, zero point energy and the force constant of the molecule. Mass of $^{14}\text{N} = 23.25 \times 10^{-27} \text{ kg}$, Mass of $^{16}\text{O} = 26.56 \times 10^{-27} \text{ kg}$.
251. The equilibrium vibration frequency of the iodine molecule is 215 cm^{-1} and the anharmonicity constant $x_e = 0.003$. What is the intensity of the hot band $\nu = 1 \rightarrow \nu = 2$ relative to that of the fundamental $\nu = 0 \rightarrow \nu = 1$, if the temperature is 300 K.
252. The fundamental vibration of H^{35}Cl is $8,667 \times 10^{10} \text{ s}^{-1}$. What would be the separation between the infrared absorption lines for H^{35}Cl and H^{37}Cl . Given $m(^{37}\text{Cl})/(m(^{35}\text{Cl})) = 1.056$.
253. The position of the lines in the fundamental band $\nu=0$ to $\nu=1$ of HCl is given by $\bar{\nu} = (2886 + 20.577m - 0.3034m^2) \text{ cm}^{-1}$, where $m = \pm 1, \pm 2$ etc. Calculate B_0 , B_1 , and B_e . Given $\alpha_e = 0.3019 \text{ cm}^{-1}$.
254. Calculate the energy in (cm^{-1}) of the photon absorbed when NO molecule goes from the state $\nu = 0, J'' = 0$ to $\nu = 1, J' = 1$. Assume that the $\nu = 0$ and $\nu = 1$ states have the same B values. Given $\bar{\nu}_e = 1904 \text{ cm}^{-1}$; $x_e = 0.00733$, $r_{\text{NO}} = 0.1151 \text{ nm}$.
255. The fundamental and first overtone transition of $^{14}\text{N}^{16}\text{O}$ are centred at 1876.06 cm^{-1} and 3724.20 cm^{-1} respectively. Evaluate the equilibrium vibration frequency and the anharmonicity constant.
256. In the vibration - rotation spectrum of HF, the rotational constant B_0 for $\nu = 0$ state is 20.6 cm^{-1} and the rotational constant B_1 for $\nu = 1$ state is 19.8 cm^{-1} . Calculate the percentage increase in bond length on going from $\nu = 0$ to $\nu = 1$ state.
257. The fundamental vibration frequency of HCl is 2989 cm^{-1} . Find the force constant of the HCl bond.
258. The equilibrium vibrational frequency of the iodine molecule is 215 cm^{-1} and the anharmonicity constant is $\chi = 0.003$. What is the intensity of the hot band $\nu = 1$ to $\nu = 2$ relative to that of the fundamental $\nu = 0$ to $\nu = 1$, if the temperature is 300 K ?
259. The fundamental band for HCl is centred at $2886 (\text{cm}^{-1})$. Assuming that the internuclear distance is 1.276 \AA , calculate the wave number of the first two lines of each of the P and R branches of HCl.
260. The normal modes of vibration of CO_2 molecules are $\bar{\nu}_1 = 1330 \text{ cm}^{-1}$, $\bar{\nu}_2 = 667 \text{ cm}^{-1}$ and $\bar{\nu}_3 = 2349 \text{ cm}^{-1}$. Evaluate the zero point energy of CO_2 molecule.
261. The wave numbers of normal modes of vibration of CO_2 are 1330 cm^{-1} , 667 cm^{-1} and 2349 cm^{-1} . Calculate the zero point energy of the molecule.
262. For the HCl molecule, the rotational constant $B = 10.285 \text{ cm}^{-1}$ for both the $\nu = 0$ and $\nu = 1$ states. If the frequency of $\nu = 0$ to $\nu = 1$ transition is at 2886.04 cm^{-1} , calculate the wavenumbers of the first two members of the O and S branches in the Raman vibration-rotation spectrum.
263. The bond length of N_2 molecule is 1.097 \AA . What would be the positions of the first three rotational Raman lines of N_2 ? Mass of $^{14}\text{N} = 23.25 \times 10^{-27} \text{ kg}$.

264. The bond length of N_2 molecule determined from Raman Spectra is 1.097×10^{-10} m. Find how far in cm^{-1} , from the exciting Raman line, the first three lines of N_2 rotational Raman spectrum are ?. Mass of $^{14}N = 23.25 \times 10^{-27}$ kg.
265. The first Raman line of H_2 appears at $346 cm^{-1}$ from the exciting line. Calculate the bond length of H_2 molecule. Mass of hydrogen atom = 1.673×10^{-27} kg.
266. With the exciting line 2536 \AA , a Raman line for a sample is observed at 2612 \AA . What is the Raman Shift?
267. The first three Stokes lines in the rotational Raman spectrum of $^{16}O_2$ are separated by $14.4 cm^{-1}$, $25.8 cm^{-1}$ and $37.4 cm^{-1}$ from the exciting radiation. Using the rigid rotor model, obtain the value of bond length.
268. A Raman line is observed at 4768.5 \AA , when acetylene was irradiated by 4358.3 \AA radiations. Calculate the equilibrium vibrational frequency that causes this shift.
269. When a substance is irradiated with 4365 \AA , radiation, a Raman line attributed to the symmetric stretching vibration is found at 4814 \AA . Calculate the fundamental frequency for this vibration.
270. Discuss in detail the rotational Raman spectrum of symmetric top molecule.
271. A substance shows Raman line at 4568 \AA , when the exciting line 4332 \AA , is used. Calculate the wavelengths of Stokes lines and Anti-Stokes lines for the same substance when the exciting line 4036 \AA , is used.
272. The exciting line in an experiment is 5650 \AA , and Stokes lines are at 5810 \AA . Calculate the wavelengths of Anti-Stokes line.
273. Irradiation of carbon tetrachloride by 4358 \AA , radiation gives Raman lines at 4400 , 4419 and 4447 \AA . Calculate the Raman shift for each of these lines in cm^{-1} .
274. Bond length of H_2 molecule is 0.7417 \AA . Determine the position of first three rotational Raman lines in the spectrum. Given, mass of $^1H = 1.673 \times 10^{-27}$ Kg.
275. A Raman line is observed at 4768.5 \AA , when acetylene was irradiated with radiation 4358.3 \AA . Calculate the equilibrium vibrational frequency that causes this shift.
276. The first rotational Raman line of H_2 appears at $346 cm^{-1}$ from the exciting line. Calculate the bond length of H_2 molecule. $^1H = 1.673 \times 10^{-27}$ Kg.
277. Light of wavelength 900 nm is incident on a material with a characteristic Raman Frequency of $20 \times 10^{12} \text{ Hz}$ results in a Stokes line. What is the shift in wavelength of the Stokes line?
278. A substance shows Raman line at 4567 \AA , when exciting line 4358 \AA , is used. Deduce the positions of Stokes and anti-Stokes lines for the same substance when the exciting line 4047 \AA , is used.
279. In the Raman spectra of $^{16}O_8$ molecule, the first three Stokes lines are separated by 14.4 , 25.8 and $37.4 cm^{-1}$ from the exciting line. Using the rigid rotator model calculate the bond length. Given Avogadro number = 6.022×10^{23} .
280. The Raman line associated with a vibrational mode which is both Raman and infrared active is found at 4600 \AA , when excited by light of wavelength 4358 \AA . Calculate the wavelength of the corresponding infrared band.
281. In the Raman spectrum of a linear triatomic molecule, the first three lines are at 4.86 , 8.14 , and $11.36 cm^{-1}$. Determine the rotational constant B and the moment of inertia of the molecule.

282. For the HCl molecule, the rotational constant $B = 10.285 \text{ cm}^{-1}$ for both the $\nu = 0$ and $\nu = 1$ states. If the frequency of $\nu = 0 \rightarrow \nu = 1$ transition is at 2886.04 cm^{-1} , calculate the wavenumbers of the first two members of the O and S branches in the Raman vibration-rotation spectrum.
283. The first-three rotational Raman lines of a linear triatomic molecule are at 4.86 , 8.14 and 11.366 cm^{-1} from the exciting Raman line. Estimate the rotational constant B and the moment of inertia of the molecule.
284. The Raman line associated with a vibrational mode which is both Raman and Infrared active is found at 4600 cm^{-1} , when excited by a light of wavelength 4358 \AA . Calculate the wavelength of the corresponding infrared band.
285. Give the classical theory of hyper Raman effect
286. The values of ν_e and $\nu_e x_e$ for upper electronic state for a diatomic gas are 439 cm^{-1} and 28 cm^{-1} and that of lower electronic state are 563 cm^{-1} and 18 cm^{-1} , respectively. The 0-0 band is observed at 37206 cm^{-1} . Calculate the wave numbers of bands (0,0), (0,1) and (1,1).
287. Draw the Fortrat parabola and explain its significance.
288. The rotational lines of a band system of electronic vibration spectra is given by $\bar{\nu} = (24762 + 25m - 2.1m^2) \text{ cm}^{-1}$ where $m = \pm 1, 2, \dots$. Deduce the value of B , B'' and the value of the band head.
289. The absorption spectrum of O_2 shows vibrational structure which becomes a continuum at 56876 cm^{-1} ; the upper electronic state dissociates into one ground state atom and one excited atom. The excitation energy measured from the atomic spectrum is 15875 cm^{-1} . Estimate the dissociation energy of ground state O_2 in kJ/mol.
290. The vibrational structure of the absorption spectrum of O_2 becomes a continuum at $56,876 \text{ cm}^{-1}$. If the upper electronic state dissociates into one ground state atom and one excited atom with excitation energy $15,875 \text{ cm}^{-1}$, estimate the dissociation energy of the ground state of O_2 in cm^{-1} and KJ mol^{-1} .
291. The rotational lines of a band system of electronic vibration spectra is given by $\bar{\nu} = (24762 + 25m - 2.1m^2) \text{ cm}^{-1}$, where $m = \pm 1, \pm 2$ etc. Deduce the values of B' , B'' and the position of band head.
292. The band origin of a transition in CO_2 is observed at 19378 cm^{-1} , while the rotational fine structure indicates that the rotational constants in the excited and ground states are $B_2 = 1.7527 \text{ cm}^{-1}$ and $B_1 = 1.6326 \text{ cm}^{-1}$. Evaluate the position of band head and wavelength.
293. The nucleus ^{11}B has $I = 3/2$ and $g_N = 1.792$. Calculate its energy levels in a magnetic field of 1.5 T .
294. A system of protons at a temperature of $25^\circ C$ is placed in a magnetic field of 2 T . What is the ratio of number of proton spins in the lower state to the number in the upper state?
295. Calculate the difference in energies of proton oriented with and against a magnetic field of strength 1.5 Tesla . What is the frequency of radiation that has a photon with this energy? $g_N = 5.5857$; $\mu_N = 5.07 \times 10^{-27}$; $h = 6.625 \times 10^{-34} \text{ Js}$.
296. Calculate the ratio of the population of the two nuclear spin states for protons in a magnetic field of 4 T at $27^\circ C$.
297. The ^{13}C NMR spectrum of a compound occurs at 10.705 MHz in a magnetic field of 1 T . What is the resonance frequency if the field applied is 3 T ?

298. A particular NMR instrument operates at 30.256 MHz. What magnetic fields are required to bring 1H and ^{13}C nuclei to resonance at this frequency. g value of 1H is 5.585 and that of ^{13}C is 1.404.
 $\mu_N = 5.051 \times 10^{-27} JT^{-1}$
299. Calculate the strength of the magnetic field to give a precessional frequency of 100 MHz for ^{17}O nucleus.
 $g_N = -0.757$, $\mu_N = 5.051 \times 10^{-27} JT^{-1}$; $I=5/2$
300. An NMR signal for a compound is found to be 180 Hz downward from TMS $[(CH_3)_4Si]$ peak using a spectrometer operating at 60 MHz. Calculate its chemical shift in ppm.
301. In a magnetic field of 1.41 T, the difference in NMR absorption frequencies for two protons is 60 Hz. Magnetic moment of proton is $14.1058 \times 10^{-27} JT^{-1}$. Estimate the chemical shift in ppm.
302. An NMR signal for a compound is found to be 180 Hz downward from TMS peak using a spectrometer operating at 60 MHz. Calculate the chemical shift in ppm.
303. The frequency separation between protons in C_6H_6 and TMS is 510.5 Hz when the field is 1.65T. What is the chemical shift?
304. A free electron is placed in a magnetic field of strength 1.5 T. Calculate the resonance frequency if $g=2.0023$.
305. A free electron is placed in a magnetic field of 2.6 T. Calculate the resonant frequency $g = 2.0027$.
 $\mu_B = 9.274 \times 10^{-24} JT^{-1}$.
306. Electron spin resonance is observed for atomic hydrogen with an instrument operating at 9.5 GHz. If the g value for the electron in hydrogen atom is 2.0026, what is the magnetic field applied? Bohr Magnetron
 $\mu_B = 9.274 \times 10^{-24} JT^{-1}$.
307. A free electron is placed in a magnetic field of 2.6T. Calculate the resonant frequency $g = 2.0027$.
 $\mu_B = 9.274 \times 10^{-24} JT^{-1}$.
308. A free electron is placed in a magnetic field of 3.6 T. Calculate the resonance frequency of $g = 2.0023$;
 $\mu_B = 9.274 \times 10^{-24} JT^{-1}$.
309. Calculate the ESR frequency of an unpaired electron in a magnetic field of 0.33 T. Given $g = 2$ and
 $\mu_B = 9.274 \times 10^{-24} JT^{-1}$
310. Electron spin resonance is observed for atomic hydrogen with an instrument operating at 9.5 GHz. What is the magnetic field applied? Given, Bohr magnetron $\mu_B = 9.274 \times 10^{-24} J/T$ and “ g ” value for the electron in the hydrogen atom is 2.0026.
311. A sodium atom ($I=3/2$, $s=1/2$) in zero field has the Hamiltonian $\mathbf{H}=\mathbf{a} \cdot \mathbf{I} \cdot \mathbf{S}$. Find the energy levels and transitions.
312. Predict the ESR hyperfine structure and obtain the frequencies when an unpaired electron interacts with three equivalent protons.
313. Calculate the recoil velocity and energy of a free Mossbauer nucleus $^{57}Fe^*$, when emitting a gamma ray of frequency 3.5×10^{18} Hz. What is the Doppler shift of gamma-ray frequency to an outside observer?
314. Calculate the recoil velocity and energy of a free Mossbauer nucleus ^{119}Sn when emitting a gamma ray of frequency 5.76×10^{18} Hz. What is the doppler shift for an outside observer?
315. A Mossbauer nucleus ^{57}Fe make the transition from the excited state of energy 14.4 KeV to ground state. What is its recoil energy and recoil velocity.

316. A particular Mossbauer nucleus has ground state spin $3/2$ and first excited state spin $5/2$. Into how many lines will the gamma ray spectrum split, if the nucleus is under the influence of a magnet field B ? Draw the energy levels and transitions

D Part

E Part