**S.T.E.T. WOMEN’S COLLEGE, MANNARGUDI**

**II M.Sc., CHEMISTRY**

**PHYSICAL METHODS IN CHEMISTRY II**

**PAPER CODE :P16CH41**

**QUESTION BANK**

**SECTION : A**

 1. Define term:-

 2. Explain term symbol :-

 3. What are States and microstates?

 4. Define Spin – orbit coupling:-

 5. What is Spin multiplicity?

 6. Write the Selection Rule for Electronic transitions:-

 7. Difference between Orgal diagram & Tanabe Sugano diagram

 8. Give any two applications of spectroscopy?

 9. Define Charge transfer spectra.

10.Define Tanabe – Sugano diagram.

11. Give the Orgal diagram of [Cu(H2O)6]2+ complex.

12. [Cu(NH3)4]+ is colourless where as [Cu(NH3)4]2+ is blue . why?

13. Define hole formalism:-

14. Difference between MCD and CD.

15. Define Racah parameters B and C

16. Mn 2+ are pale in color explain.

17. [ FeF6]3- is colorless where as [CoF6]3- colored why?

18. Define faraday effect:-

19. Explain circular Birefrigence:-

20. Define JJ coupling:-

21. Discuss the electronic spectrum of [V(H2O)6]2+

22. Define band shape?

29. How the hunds rule used in determination of term symbol in ground state

30. [Ti(H20)6]2+ is purple in color. Explain.

31. Describe the CT spectrum of Mno4- have no d-d transitions

32. Find the ground state term symbol for d5 configuration.

33. Deduce the term symbol for d4 case.

34. The electronic spectrum of [Ti(H2O)6]3+ is broad.Explain.

35. [CU(CN)6]3- is high CFSE than that [CO(NH3)6]3+

36. [Ni(H2O)6]2+ is high CFSE than that [Ni(NH3)6 ]3+

37. CT bands are more intense than d-d transition why?

38. Define near IR and far IR?

39. Write the Principle of IR spectroscopy?

40. What are the types of vibrations?

41. Define finger print region?

42. Explain Fermi resonance?

43. What are the factors affecting vibrational frequency in IR?

44. Define reference beam and sample beam?

45. Explain the types of hydrogen bonding in IR spectroscopy?

46. Some of the fundamental vibrations are infra red active while others are not. Explain

47. How will you distinguish between cis and trans cinnamic acid?

48. Explain fundamental vibration and overtones?

49. Define Raman scattering?

50. Explain stokes and Anti stokes lines?

51. Define Rayleigh line?

52. What is meant by Raman frequency?

53. Explain Raman spectrum?

54. What are the characteristics of Raman lines?

55. Explain polarized and Depolarized light?

56. What is the conditions for substance to be Raman active?

57. Explain the rule of mutual exclusion?

58. Explain intensity of Raman lines?

59. Describe the effect of temperature on Raman lines?

60. Define Raman effect?

61. What are the Application of IR?

62. Write the Advanages of Raman spectroscopy over IR?

63. Indicate some applications of mass spectra on inorganic field.

64. Define precessional frequency?

65 Define Shielding and Deshielding of proton?

66. Define chemical shift?

67. Compare the NMR spectrum of

 1. CH3 – CH2 – F &

 2. CH3 – CH2 – Cl

68. How will you distinguish inter and intra molecular hydrogen bonding by NMR spectroscopy?

69. What are the solvents are used in NMR?

70. Sketch the NMR of 1:1:2 tri chloro tri chloro ethane?

71. How many signals for 2- chloro propene?

72 Sketch NMR spectrum of 1:1 tri fluro 1,2 dichloro ethane?

73. What is Spin – spin coupling?

74. Define Coupling constant:

75. NMR spectrum of 1-bromo 3-chloro propane :

76. What is meant by (n+1) rule?

77. Aldehyde proton appear much downfield in the NMR spectroscopy? Explain

78. What is Geminal coupling , vicinal coupling and long range coupling?

79 What is spin decoupling or double Resonance ?

80. Sketch the NMR spectrum 1-bromo – fluoro ethane :

81. Predict the number of signal in NMR?

82. **13C** NMR is active while **12C** is not?

83. Predict the numbers of signals in NMR of p- nitro toluene :

84. Why TMS is used as a reference in NMR spectroscopy:

85. In a given organic compound two kinds of protons exhibit signals at 50HZ and 200HZ using a 60MHZ instrument . what would be their equivalent positions using 10 MHZ spectrometer?

86. What is spin – spin splitting?

87. predict the number signals in NMR spectrum of cinnamaldehyde?

88. predict the number of signals and their multiplet for the PMR:

89. Halogen nuclei have large Dipole moment but still there are practically non magnetic ,where as 14N and 2H are magnetic for the purpose it high resolution NMR spectroscopy explain:

90. How will you distinguish cis and trans stilbene by means of NMR spectroscopy?

91. Aldehyde proton appear much downfield in the NMR spectroscopy? Explain:

92. Acetylene are more shielded than Ethylene protons explain:

93. Define contact shift

94. Explain pseudo contact shift:

95. How many lines are expected in the 31P NMR of HP(OH2) and H2PO(OH)draw this :

96. Indicate some lanthanide shift reagents and give their significance:

97. Sketch the 19 F NMR ClF3 which is ‘T’ shaped?

98. Define EPR spectroscopy:-

99.What is Zeeman effect?

 100. What is spin lattice relaxation?

 101. Define first order Zeeman effect

 102. What is Second order Zeeman effect?

 103. Define magnetic susceptibility:

 104. What is meant by TIP?

 105. Write any two consequence of kramer's rule?

 106. Define spin Hamiltonian:-

 107. Why water & alcohol are not suitable solvent for the ESR studies:-

 108. Define SOC?

 109. Discuss the magnetic properties of lanthanides and actinides:-

 110. Define Magnetic susceptibility? (k)

 111. Explain hyperfine couplings in isotropic system?

 112. Write the McConnell equation?

 113. What are the factors affecting g-value ?

 114. What do you mean by spin density?

 115. What is Kramer’s degeneracy:-

 116. Difference between diamagnetism and Para magnetism:-

 117. Define zero field splitting:-

 118. What is Dipole-Dipole interaction?

 119. Define stable and unstable paramagnetic substance:-

 120. Difference between ESR and NMR:-

 121. What are the types of magnetism.

 122. What is Quadruple moment? Give examble

 123. What is nuclear Quadruple resonance?

 124. Define nuclear quadruple coupling constant.

 125. What are the methods for the detection of NQR frequencies?

 126. NQR of solid sicl4 is four line spectrum explain.

 134. What is the use of quadrupole resonance?

 135. Write a note on the results of 35cl resonance on group

 III halids group, III Trihalides

136. Write a NQR spectrum of group IV halides:-

137. MB spectroscopy is a complementary tool to other techniques such as NMR , ESR and NQR. explain .

138. Define isomer shift ?

139. Ilustrate the decay scheme of 57co showing the energy Levels in 57fe 119sn.

140. What are the γ-rays nucleus and Sources are used in MB spectroscopy?

141. Define Isomer shift?

142. Discuss (IF6)- MB spectrum?

143. Which effects can give rise to multiple lines in the NQR spectrum

144. List the characteristics of quadrupolar nuclei.

145. How will you distinguish high spin Fe(II) &Fe(III) complexes by MB spectra?

**SECTION : B**

1. What are microstates? Deduce all microstates for P2 configuration.
2. The complex [Cr(H2O)6]3+ shows three spin allowed transitions at 17400 cm-1, 24600 cm-1 and 37800cm-1 evaluate 10 Dq and B1.
3. With suitable examples show how IR spectroscopy is useful in the study of
4. Inter and intra molecular hydrogen bonding.
5. Identification of terminal and bridging CO of poly nuclear carbonyls.
6. Group theoretically analyzes IR and Raman stretching mode in metal carbonyls.
7. Enumerate the principle of NMR spectroscopy discuss in the study of intra molecular rearrangement.
8. Write a note on the use of shift reagents in NMR spectra.
9. Discuss the factors affecting the G value of an electron on ESR spectrum.
10. Explain briefly spin cross over in coordination compounds.
11. The moss Bauer spectra of [Fe (CN)5NO]2- shows a very large quadruple splitting while that of [Fe(CN)6]4-does not exhibit any splitting at all. Why?
12. What structural information in provided by NQR in the study of group III halides?
13. Apply group theory and formulate the selection rules for electronic transitions.
14. What is john – Teller effect? How does it affect the electronic spectrum of transition metal complexes?
15. Explain the term ‘Molecular Fragmentation’ with a suitable example.
16. With suitable illustration explain how complexes are characterized by IR spectroscopy.
17. Explain NMR study of paramagnetic molecules.
18. What do you mean temperature independence paramagnetism?
19. How are structure and bonding in tin complexes studied which the help of Mossbauer spectroscopy?
20. Discuss the effect of filed gradient and magnetic field upon quardrupole energy levels.
21. Write notes on

i. Charge transfer spectra and

ii. Spectro chemical series.

1. Discuss the electronic spectra of [COCl4]2- and [Ni(H2O)6]2+.
2. Explain the priv[ciple and application of resonance Raman spectroscopy.
3. Account for the following infrared data:

 Complex υ Cm-1

1. [Fe(CN)6]4- 584
2. [Fe(CN)6]3- 505
3. [CO(CN)6]3-  564
4. [Cr(CN)6]3-  462
5. [Mn(CN)6]3- 514
6. Explain how NMR is useful in evaluating rate of a reaction.
7. Cyclohexene gives a proton NMR spectrum containing only one signal at room temperature. However at low temperature it produces a very complex spectrum explains.
8. Explain the EPR spectrum of d5 high spin and d8 cases.
9. The 14N resonance of a compound showed 3 lines at 5.997, 3.501 and 2.496 MHZ. Calculate the quadrupole coupling constant e2 qQ/h and η.
10. Calculate the recoil velocity and energy of the free Mossbauer nucleus 119Sn when emitting a γ – ray of frequency 5.76 × 108 Hz. What is the Doppler shift of the γ – ray frequency to an outside observer?
11. Discuss the splitting of D and F terms under the influence of weak Voct and Vtet.
12. Discuss the electronic spectra of [Fe(Cl4)]2 and [V (H2O)6]3+.
13. Rationalize the following data:

 Species CO stretching frequency / CM-1

1. Co 2145
2. Mo(co)6 2000
3. Mo(co)3  1855
4. (NH3)3
5. Explain the molecular fragmentation pattern and its application in inorganic mass spectroscopy.
6. 17O NMR spectrum of [W6O19]2-  consist of three signals which is a singlet. These signals have the intensity ratio 12:6:1 what structural features are evident from this spectrum.
7. Predict the number of spectral lines for Cr(H2O)62+ complex. Indicate how zero-field spitting and Kramer’s degeneracy applied to this complex.
8. Explain the epr spectrum of d5 low spin and d6 case .
9. Calculate the Doppler velocity corresponding to the natural line width of the γ ray emission from14.4Kev excited state of 57Fe nucleus having a half life of 9.8×10-8 s.
10. How are the co-ordination of sulphate ligand and its dentality in the complex evaluated from IR data.
11. Calculate the energy difference between two magnetic dipole states in the case of i)Electron ii)proton at 10,000 gauss magnetic field.
12. Predict and sketch 1H and 19F NMR spectra of 1bromo 1fluoroethane(each being recorded in the same magnetic field.)
13. Explain the following terms

 i) Base peak

 ii) Isotopic peak

 iii) Parent peak

 iv) FAB mass spectrometry

 v) EI mass spectrometry

 40. Illustrate the effect of zero fields splitting on the EPR spectrum citing octahedral Mn2+ complex. The product obtained from the reactions of ferrous sulphate and potassium ferrocyanide gives rise to the spectrum below, Interpret the spectrum.

41. Write a note on haloketone and octant rules.

42. What are the different types of CT spectra. Illustrate with suitable example.

43. Explain the spectra of Ti(H2O)63+ and Cu(H2O)62+ with orgel diagram.

44. Discuss the effect of distortion and spin orbit coupling on electronic of inorganic complexes.

45. Highlight the importance of IR and Raman spectroscopy in the structure analysis of nitrate per chlorate ClF3 and N2O, Clo4.

46. Discuss hoe the symmetry of the complex affects the number of absorption bands in IR.

47. What are the principles of Raman spectroscopy give two applications, to inorganic compounds.

48. Write a note on Group vibration and its limitations.

49. i) Distinguish between satellite peaks and spinning side bads.

 ii) Spin spin relaxation and spin lattice relaxation.

50. Indicate hoe the thermodynamic parameters can be obtained by recording the NMR spectrum of different temperature.

51. Briefly discuss the effect of equadrupolar nuclei om the 1H NMR spectra.

52. Predict and sketch the 31P NMR spectrum of i) H3PO3 ii) P3N3Cl4F2.

53. Discuss the factors influencing coupling involving 1H – 1H and 1H – 31P and 1H – 13C systems.

54. Explain how the magnetic moments can be determined?(OR) Describe G way balance method.

55. Distinguish between first order and second order Zeeman effects . Describe the magnetic properties of free ions.

56. Discuss the EPR spectrum of Cu(II) complexes.

57. Discuss the quenching of orbital angular momentum for A and E terms.

58. Mention the properties of lanthanides and Actinides.

59. What is Zero field splitting? Explain Krammer’s degeneracy.

60. Discuss the EPR spectrum of Cu(II) complex of 5 – chloro salicyaldoxim.

61. The 121Sb spectrum of solid SbF5 does not indicate any resolved quadrupole splitting. Explain.

62. Explain how the presence of hydrogen bonding in studies with NQR.

63. Give an account of NQR spectrum of K2SeCl6.

64. Discuss the effect of co – ordination on ligand vibration.

65. Write the combined use of IR and Raman spectroscopy in the structural elucidation of the following.

 i) N2O ii) NO3- iii) ClF3

66. Define chemical shift? Explain the factors affecting chemical shift.

67. Explain pseudo contact shift in NMR.

68. Describe the magnetic hyperfine interaction in MB spectroscopy.

69.Write a note on term symbols.

70. Establish that MB spectroscopy is a complementary tool to other spectral techniques like EPR, NMR and NQR.

**SECTION : C**

1. Write an essay on charge transfer spectra.
2. Discuss the principles and presentation of Raman spectroscopy.
3. Discus about the NMR of paramagnetic molecules.
4. Discuss the theory and applications of EPR spectroscopy.
5. Write the principles and application of NQR spectroscopy.
6. Write the structural elucidation of metal complexes of the following using group vibration i) urea ii) Thiourea iii) Cyanide iv) Thiocyanate v) Nitrate.
7. Discuss the study of fluxional behavior of molecules.
8. Discuss the following i) isotropic shifts ii) contact and pseudo contact interactions.
9. Discuss the effect of the isotropic substitution on the vibrational spectra molecules.
10. Discuss the steps in the evaluation of Dq and A Illustrate with an NI complex.
11. What are the different types of CT spectra. Illustrate with suitable examples.
12. How is IR spectroscopy and used to explain the vibrational spectra of metal carbony?
13. Discuss the [principles and application of resonance a Raman spectroscopy.
14. Discus the EPR spectrum of Cu(II) complex.
15. Discuss the quenching of orbital angular momentum for A:E and T terms.
16. Write note on i) Significance of 10Dq ii) Magnetic circular dichorism iii) Charge transfer spectra.
17. Highlight the importance of IR and Raman spectroscopy in the structure analysis of nitrate per chlorate ClF3  and N2O.
18. Define chemical shift and coupling constant. Explain the factors that determine the magnetic of these parameters.
19. Explain the consequences of magnetic hyper tic interaction in Mossbauer spectroscopy. Indicate how the crystal symmetry and magnetic structure can be analyzed using Mossbauer spectroscopy.
20. Explain briefly SCO in co – ordination compounds
21. Discuss the application of EPR in Cu(II) containing molecule.
22. Explain the importance of IR and Raman spectroscopy in the structural analysis of urea, thiocyanate N2O,ClO.4.
23. How IR spectroscopy is useful in the study of inter and intra molecular hydrogen bonding.
24. Explain the concept of ORD and CD – Explain hoe they are used to study the chirality of metal complexes.
25. Explain with suitable example how ORD and CD are useful in detrerminating the absolute configuration of metal complexes.
26. Explain the electric spectrum of tetrahedral complexes of CO(II) with the help of orgel diagram? A tetrahedral complex of CO(II) shown bands at 5800 and 15000cm-1 calculate B’ B and 10Dq.
27. Explain use of IR spectrum in analyzing the SlC of metal carbonyls with respect to their geometry and bonding.
28. Discuss the effects of the isotopic substitution on the vibrational spectra of molecules.
29. How are complexes characterized by IR spectral data? Illustrate with two examples.
30. Explain the pseudo contact shift in NMR.
31. Distinguish between first order and second order Zeeman effects. Describe the magnetic properties of free ion.
32. Discuss the selection rules for electronic transitions in term of group theory.
33. Write briefly on the application of optical rotatary dispersion studies in solving the configurational and conformational problems associated with cyclic compounds possessing suitable chromophores
34. What is the principle involved in mass spectrum? Explain the fragmentations of ethylamine.
35. Explain how EPR spectral measurements are useful in studying JT effects in Cu(II) complexes.
36. Compare the temperature dependence of paramagnetic, ferromagnetic and anti ferromagnetic substances.
37. How does MossBauer spectroscopy help the study of structure and bonding in tin complexes?.

 Give an account of NQR spectrum of K2SeCl2.