STELLA MARIS COLLEGE (AUTONOMOUS) CHENNAI-86
(For candidates admitted during the academic year 2009–2010 & thereafter)

SUBJECT CODE: CH/PC/MS34

M.Sc. DEGREE EXAMINATION, NOVEMBER 2011
BRANCH IV- CHEMISTRY
THIRD SEMESTER

REG.NO ……..

COURSE : CORE
PAPER : MOLECULAR SPECTROSCOPY
TIME : 30 MINUTES **MAX.MARKS : 20**

SECTION – A **(20x1=20)**

Answer all the questions:

I Choose the correct answer:

1. The ΔE for a typical ultraviolet wavelength of 200 nm is
   a) 9.9 x 10^{-12} erg b) 9.9 x 10^{-14} erg c) 9.9 x 10^{-16} erg d) 9.9 x 10^{-10} erg
2. Phosphorescence is
   a) red heat emission b) black body emission
   c) ultraviolet emission d) visible light emission
3. Bathochromic shift is
   a) short wavelength shift b) long wavelength shift
   c) low intensity shift d) high intensity shift
4. The special instrumental feature present in FT-IR is
   a) gratings b) beam splitter c) optical balance d) thermostat
5. The expression to calculate m/e is
   a) $B^2r^2/2V$ b) $B^2V^2/2r$ c) B^2r^2/V d) $2B^2r^2/V$
6. The CO_2 molecule is
   a) only IR active b) only Raman active
   c) both IR and Raman active d) neither IR nor Raman active
7. The IR vibrational stretching frequency for C=N is
   a) 1830 cm^{-1} b) 1980 cm^{-1} c) 1350 cm^{-1} d) 1650 cm^{-1}
8. The spin-spin splitting pattern for O_2N-C*H*$_2$-C**H**$_2$-C$\underline{H}_2$-Cl is
   a) *3*,**5**,$\underline{2}$ b) *3*,**5**,$\underline{3}$ c) *2*,**6**,$\underline{3}$ d) *3*,**3**,$\underline{3}$
9. The identification of correct species from mass spectral pattern is helped out by
   a) Pascal's table b) Beynon's table c) Clarke's table d) none of the above
10. The ^{13}C NMR spectrum produces singlets for various types of carbons due to
    a) coupling of protons b) spin-spin splitting
    c) shift reagents d) noise decoupling

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II Fill in the blanks:

11. The number of normal modes of vibrations calculated for linear molecule of N atoms is _____.
12. The unit for molar extinction coefficient is _____..
13. An example for a shift reagent is _____.
14. The source of IR radiation is _____.
15. The reduced mass value of C and N is _____.

III Answer the following in one or two lines:

16. State Franck Condon principle.

17. Write the selection rule for microwave spectrum.

18. What are overtones in IR?

19. What is spin decoupling?

20. How mass spectral fragments are formed by retro Diel's Alder rearrangement?

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COURSE : CORE
PAPER : MOLECULAR SPECTROSCOPY
TIME : 2½ HOURS **MAX.MARKS : 80**

SECTION – B **(5 x 8 = 40)**

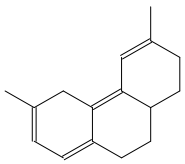
Answer any five questions:

1. a) Draw the rotational vibrational spectrum of CO molecule. (3)
   b) How the fundamental vibrational frequencies are affected by vibrational coupling and H-bonding? Explain with suitable examples. (5)

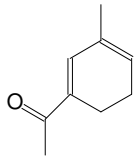
2. a) What is the importance of molar extinction coefficient in UV-visible spectroscopy? (4)
   b) How is Raman spectroscopy complementary to IR spectroscopy? (4)

3. Calculate the λ_{max} of the following compounds. (4+4)

a)

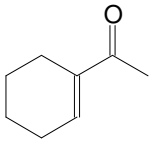


b)



4. Predict various mass spectral fragmentation patterns for alcohols and ketones. (4+4)

5. Predict the possible IR and UV spectral pattern for the following compound. (4+4)



6. Write a short note on the following. (3+2+3)
   a) Effect of polar and non-polar solvents on n $\rightarrow \pi^*$ transition
   b) Pascal's triangle
   c) Bond angles altering IR frequencies

7. What are the factors affecting the coupling constant? Explain any two of them with example. (4+4)

8. Predict the multiplicities of NMR signals of the following compounds. (3+2+3)
   i) 1,1,3-trichloropropane
   ii) di-isopropylether
   iii) 2-methylbutanone

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SECTION – C (2 x 20 = 40)

Answer any two questions:

9. a) Calculate the frequency of the stretching vibration of C≡C. ($k = 15 \times 10^5\ gs^{-2}$) (5)
   b) Why is $K_2Cr_2O_7$ colored? Explain the reason. (5)
   c) Explain the significance of re-emission of energy of an excited molecule with suitable diagram. (10)

10. a) From the following mass spectral pattern, identify the compound. Give suitable explanation for the fragments formed. (6)

m/e	12	13	14	15	28	29	30	31	32
Relative Abundance	0.33	0.72	2.4	13	6.3	64	3.8	100	66

   b) What are the limitations of microwave spectroscopy? (4)
   c) What are the factors influencing chemical shifts in NMR? Explain any two in detail with examples. (10)

11. a) Write a short note on chemical analysis using UPES. (5)
   b) How is solution NMR different from solid state NMR spectroscopy? Write any one application of solid state NMR. (5)
   c) From the following spectral data, identify the structure of the compound. The molecular formula of the compound is $C_7H_{14}O_2$. Give suitable explanation for your prediction. (10)

   UV-visible: 280 nm
   IR (cm^{-1}) : 3000, 1705, 1370, 1210, 1080
   Mass m/e (Relative abundance) : 130 (0.2), 115 (18), 100 (10), 73 (83), 43 (100)
   H NMR (ppm): 1.3 (s, 12 squares), 2.1 (s, 6 squares), 2.5 (s, 4 squares), 3.2 (s, 6 squares)
   C NMR (ppm): 24 (double intense), 32, 50, 54, 74, 208

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