

D2ACH2104

(3 Pages)

Name.....

Reg.No.....

SECOND SEMESTER M.Sc. DEGREE EXAMINATION, APRIL 2022

(Regular/Improvement/Supplementary)

CHEMISTRY

FCHE2C08: MOLECULAR SPECTROSCOPY

Time: 3 Hours

Maximum Weightage: 30

Section A: Short answer questions. Answer any *eight* questions. Each carries 1 weightage.

1. Explain the relevance of Heisenberg's uncertainty principle in predicting the line width of spectrum.
2. What is the effect of substituting a hydrogen atom by a deuterium atom in hydrogen molecule on rotational constant **B**.
3. Why are the Stoke's lines more intense than Anti-Stoke's lines in Raman spectra?
4. Nitric Oxide shows a Q branch in the vibration-rotation spectrum. Why?
5. What is meant by Cotton effect?
6. Write Mc Connel equation and explain the terms.
7. Predict the number of proton NMR signals in *N,N*-Dimethyl formamide.
8. Mention the types of absorption and intensity shifts in UV spectroscopy.
9. Explain the concept of pre-dissociation with example.
10. How will you distinguish methyl propionate from ethyl acetate by ¹H NMR spectroscopy?
11. State and explain Karplus relationship.
12. Differentiate between HMBC and HMQC spectra.

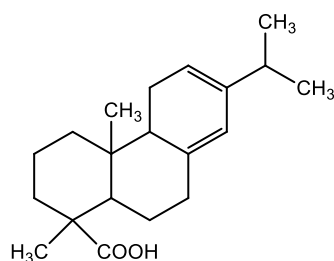
(8×1 = 8 weightage)

Section B: Short essay questions. Answer any *four* questions. Each carries 3 weightage.

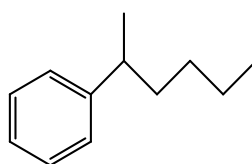
13. What is meant by 'g factor' in ESR spectroscopy? Discuss the hyperfine splitting shown by NH radical in its ESR spectra.
14. What is Nuclear Overhauser Effect (NOE) and explain its significance.

(P.T.O.)

15. Predict λ_{\max} for the following compound. Justify your answer.



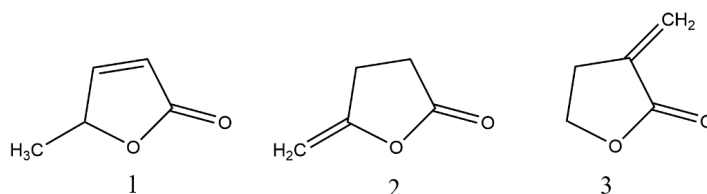
16. Discuss the major fragmentation pathway of the following molecule.



17. Predict the proton decoupled ^{13}C NMR and DEPT spectrum of the following compound.



18. Explain the effect of relative magnitudes of spin-spin coupling and chemical shift on the spectrum of AB type molecule.
19. Predict the order of stretching frequency (in cm^{-1}) from IR spectra of the carbonyl group of following compounds. Discuss.

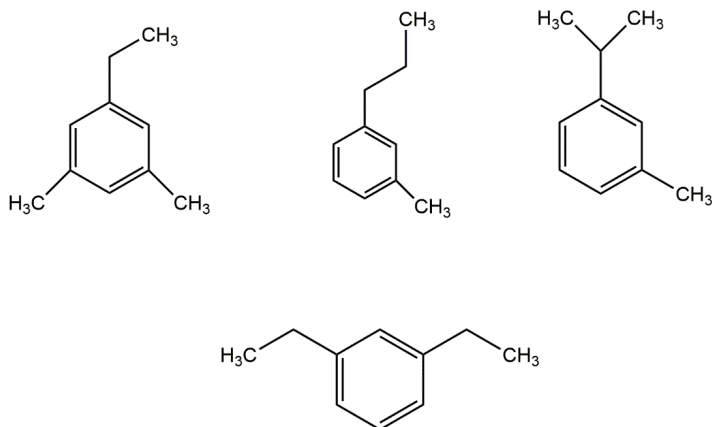


(4×3 = 12 weightage)

Section C: Essay questions. Answer any two questions. Each carries 5 weightage.

20. (a) Explain the theory and applications of Mossbauer spectroscopy by choosing different coordination complexes.
- (b) Discuss electronic spectra of conjugated molecule using particle in a box model.
21. Write note on:
- (a) Stark effect (b) Franck - Condon principle
- (c) 2D NMR COSY (d) Kramer's theorem (e) Resonance Raman spectroscopy.

22. (a) Discuss the factors which determine the width and intensity of spectral lines.
- (b) Among the following isomers of $C_{10}H_{14}$, predict the isomer that can be identified uniquely by mass spectrometry. Justify your answer.



23. (a) Deduce the structure and stereochemistry of the compound from the following spectral data. Explain the pattern of each and every signal with suitable explanation.
- (i) UV: 284nm, 308nm.
 - (ii) IR: 1690 cm^{-1} .
 - (iii) $^1\text{H NMR}$ - δ (ppm): 6.7(dd, $J=16\text{ Hz}$, 8 Hz , 1 H) , 7.40 (m, 5 H), 7.45 (d, $J=16\text{ Hz}$, 1 H), 9.75 (d, $J=8\text{ Hz}$, 1 H).
 - (iv) $^{13}\text{C NMR}$ - δ (ppm): 128.2, 128.3, 128.8, 131.0, 134.0, 152.0, 193.0.
 - (v) Mass- m/z : 132, 131, 103.
- (b) Explain first order and non-first order NMR spectra.

(2×5 = 10 weightage)