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Reg. No.....

Name.....

M.Sc. DEGREE (C.S.S.) EXAMINATION, FEBRUARY 2021

Third Semester

Faculty of Science

Branch : III—Chemistry

AN3C12/AP3C12/CH3C12/PH3C12/PO3C12—SPECTROSCOPIC METHODS IN CHEMISTRY

(Common to all Branches of Chemistry)

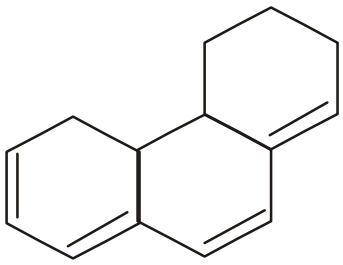
[2012—2018 Admissions]

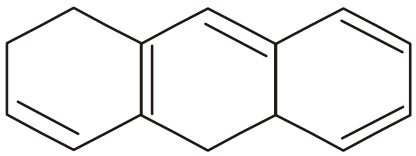
Time : Three Hours Maximum Weight : 30

Section A

Answer any **ten** *questions.*
Each question carries a weight of 1.

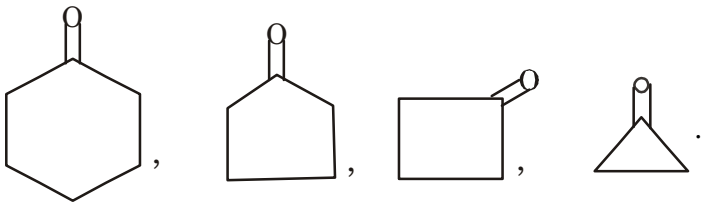
1. State and explain axial Haloketone rule.
2. Explain the phenomenon 'Circular birefringence'.
3. How is intramolecular and intermolecular hydrogen bonding distinguished using IR spectra .
4. What is Fermi Resonance ? How the corresponding peaks are identified in IR spectra.
5. Explain the term diamagnetic ring current as used in NMR spectroscopy.
6. What are shift reagents ? How it is useful in interpreting complex NMR spectra ?
7. Explain the application of McLafferty rearrangement in Mass spectra.
8. What is nitrogen rule ? Explain its use in determining the molecular mass.
9. How the presence of Chlorine and Bromine is indicated in mass spectra.
10. Calculate the λ_{max} values for the following compounds :

(a)  .

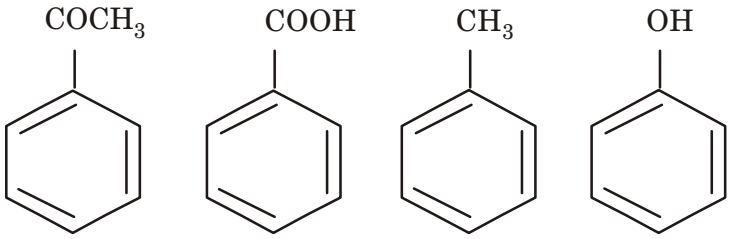
(b)  .

Turn over

11. Arrange the following carbonyl compounds in the increasing order of stretching frequencies in IR spectra :



12. Predict the base peak in the mass spectra of the following compounds :



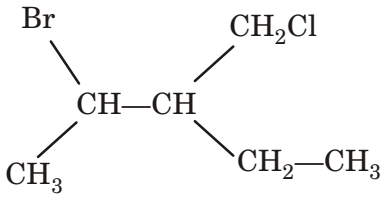
13. How is a π to π^* and n to π^* transitions distinguished in UV spectra. Explain using suitable examples.

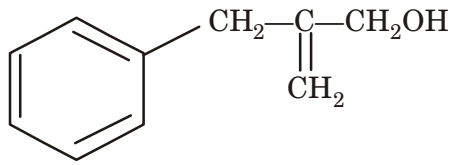
(10 × 1 = 10)

Section B

Answer any **five** *questions.*
Each question carries a weight of 2.

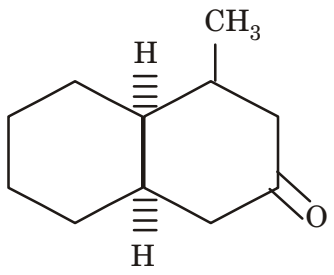
14. Sketch the approximate ^{1}H NMR and ^{13}C NMR spectrum of the following molecules :

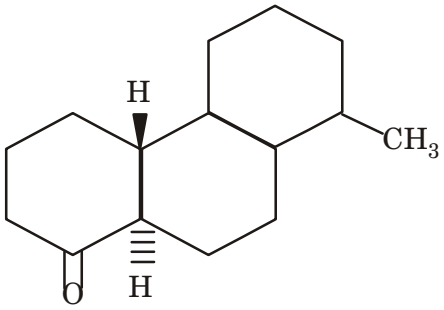
(a) 

(b) 

15. What are Cotton curves ? What are its uses ? Explain stating specific examples.

16. Explain octant rule ? Predict the sign of optical rotation in the following molecules :

(a) 

(b) 

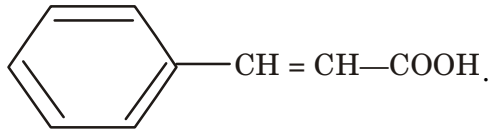
17. Sketch the H-H HOMOCOSY of : (a) 2-Bromopropane ; and (b) Isopropanol.

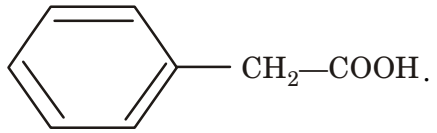
18. What is NOE ? What is the use of an NOE spectrum in structure elucidation ?

19. Give Karplus equations. Draw the Karplus curves and explain its important features.

20. Describe briefly the important methods used in the ionisation process in mass spectral Studies. Compare the advantages of the different methods.

21. Predict the signal patterns in DEPT-90 and DEPT-135 spectra of the following :

(a) 

(b) 

(5 × 2 = 10)

Section C

Answer any **two** *questions.*
Each question carries a weight of 5.

22. Write briefly on the following : (a) LC-MS ; (b) HETROCOSY ; and (c) ORD.

23. Give the spin-spin splitting patters of the following types in NMR spectra :

(a) AX. (b) ABC.

(c) A_2X_3.

Turn over

24. An organic compound A (molecular formula : $C_9H_{10}O_2$) exhibits the following spectral data IR : 1745 cm^{-1} (s) ; 1225 cm^{-1} (br,s) ; 749 cm^{-1} (s) ; 697 cm^{-1} (s).

    UV : λ_{max} at 268 nm, 264 nm, 262 nm, 257 nm.

    ^{1}HNMR : δ 1.96 (3H, singlet) ; 5.00 (2H, singlet) ; 7.22 (5H, singlet). Deduce the structure of the compound A.

25. An organic base with molecular formula $Cl_4H_{19}N$ shows the following spectral data IR : 3022 cm^{-1} (m) ; 1600 cm^{-1} (m) ;1510 cm^{-1} (m) ; 1680 cm^{-1} (w) ; 750 and 695 cm^{-1} (m).

    UV : λ_{max} at 222 nm, €$_{max}$, 20,400 ; 210 nm, €$_{max}$ 20,000.

    ^{1}HNMR : δ 2.85 (3H, singlet) ; 1.5 (3H, singlet) ; 2.0 (4H, multiplet) ; 1.65 (4H multiplet) 6.55 (3H, multiplet) and 7.05 (2H multiplet). Deduce the structure of the compound A.

$(2 \times 5 = 10)$