(Pages : 3)

Reg. No. :

Name :

Third Semester M.Sc. Degree Examination, February 2015 Branch : Chemistry CH/CL/CA 232 : ORGANIC CHEMISTRY - III (2013 Admission Onwards)

Max. Marks: 75

Time : 3 Hours

SECTION - A

Answer **any two** among (a), (b) and (c) from each question. Each sub-question carries 2 marks.

- a) Give the names of two commonly used solvents in IR spectroscopy. Water and ethanol are not used commonly in IR spectroscopy. Give reason.
 - b) λ max values of the two geometrical isomers of stilbene (C₆H₅CH = CHC₆H₅) are 278 and 294. Correlate the isomers with the corresponding λ max and give reasons.
 - c) Give the base peak or the most abundant peak in the mass spectrum of toluene.
- 2. a) Account the fact that the δ value of an aromatic H(6 8.5 ppm) is higher than a vinylic H (4.6 5.9) in PMR spectrum.
 - b) Illustrate the statement "Chemically equivalent but magnetically non-equivalent protons" with suitable example.
 - c) Give one reason why 13 C NMR is less sensitive than 1H NMR.
- 3. a) Discuss the term "hydrophobic interactions" with respect to protein structures.
 - b) What are molecular tweezers ? Give any two applications.
 - c) Explain supramolecular liquid crystals.

(2×10=20 Marks)

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- 4. a) Illustrate retrosynthesis with an example.
 - b) Differentiate in-silico and in-vitro analysis of drugs.
 - c) Predict the sign of the constant ρ in the Hammett equation for the reaction, $Ar - H + NO_2^+ \rightarrow Ar - NO_2 + H^+$
- 5. a) Write any four basic principles of green chemistry.
 - b) What types of vessels are used in microwave synthesis and give reasons?
 - c) What are ionic liquids ?

SECTION – B

Answer either (a) or (b) of each question. Each question carries 5 marks.

6. a) Explain how a polar solvent shifts the wavelengths of

i) $\pi \rightarrow \pi^*$ and

- ii) $n \rightarrow \pi^*$ transitions.
- b) Write the fragmentation pattern to account the major peaks of each of the following compounds.
 - i) $CH_3CH_2COOCH_3$; m/z = 57, 59 and 88
 - ii) $CH_3CH_2NHCH_2CH_2CH_3$; m/z = 30, 44, 58, 72 and 87
- 7. a) Account the following :
 - i) In PMR spectra, δ value of the olefinic protons of cis-stilbene is at 6.55 ppm, whereas the δ value of the olefinic protons of trans-stilbene is at 7.10 ppm.
 - ii) 1, 2 dibromoethane and cyclohexane have single sharp signals in PMR although they have conformationally different Hydrogens.
 - b) Deduce the structure of a compound C8H8O which gives 1H NMR data as δ 7.28 (5H, multiplet), 2.8 (2H, doublet), 9.78 (1H, triplet) ppm.
- a) Discuss briefly the importance of molecular recognition in DNA and protein structure.
- b) Write short notes on the following types of interactions in molecular recognition
 - i) π -stacking
 - ii) hydrogen bonding

- 9. a) Explain briefly on "combinatorial organic synthesis".
 - b) "Natural products have played a key role as a source of novel drugs or lead compounds for the development of drugs". Justify this statement briefly with suitable examples.
- 10. a) What is sonochemical synthesis ? Explain any two applications.
 - b) Write short notes on :
 - i) Green solvents
 - ii) Scavenger resins

(5×5=25 Marks)

SECTION-C

Answer any three questions. Each question carries 10 marks.

- 11. Describe briefly the major ion production techniques in mass spectrometry.
- 12. Predict the number of signal, relative chemical shifts and multiplicities in the PMR spectrum of the following compounds.
 - i) (CH₃)₂CHCOCH₃
 - ii) BrCH₂CH₂CH₂Br
 - iii) p-CH₃CH₂OC₆H₄NH₂
 - iv) C₆H₅CH₂CH₂CH₂Br
- 13. Write short notes on the following synthetic molecular receptors.
 - i) Cryptands
 - ii) Calixarenes
 - iii) Cyclophanes
 - iv) Cyclodextrins
- 14. Write the synthesis of

Chloramphenicol and phenobarbital

15. Explain in detail with examples of microwave synthesis as a green technology.

(3×10=30 Marks)

(Pages: 3)

Reg. No. :

Name :

Third Semester M.Sc. Degree Examination, January 2016 **Branch : Chemistry** CH/CL/CA 232 : ORGANIC CHEMISTRY - III (2013 Admission Onwards)

Time : 3 Hours

SECTION - A

Max. Marks : 75

Answer any two among (a), (b) and (c) from each question. Each sub-question

- 1. a) How IR spectroscopy is used to distinguish concentrated solutions of C_2H_5OH and CH_2OHCH_2OH since both give O-H stretching band at 3350 cm⁻¹?
 - b) Aniline absorbs at λ max 280 nm, but on acidification, it is shifted to 203 nm –
 - c) How will you identify the mass spectrum of a compound containing one bromine atom?
- 2. a) Account for the fact that [18] annulene has two signals (8.9 ppm and -1.8 ppm)
 - b) What is Nuclear Overhauser Effect (NOE)?
 - c) Predict the number of signals in the proton spin decoupled 13C spectrum of allyl bromide $CH_2 = CHCH_2Br$.
- 3. a) What are cyclophanes?
 - b) Explain the term " π -stacking".

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- c) Give two examples of clathrate hydrates of gases and mention their uses.
- 4. a) Give an example for solid supported automated organic synthesis.
 - b) Differentiate in-vitro and in-vivo analysis of drugs.
 - c) State the Hammett equation and explain the constants σ and ρ .

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- b) CO₂ is an excellent 'green' solvent as well as a greenhouse gas. Give reason. 5. a) Define "biocatalysts" and "atom economy". (2×10= 20 Marks)

 - c) What are scavenger resins ? Give one example.

SECTION-B

Answer either (a) or (b) of each question. Each question carries 5 marks. 6. a) Using Woodward-Fieser rule, calculate the λ max of the following compounds.

- - i) $CH_3CH_2C(CH_3) = CHCOCH_3$
 - ii) $CH_3 CH_2 C (=CH_2) COCH_3$



- iv)
- b) i) Explain McLafferty rearrangement with examples.
 - ii) Show the typical fragmentation pattern in benzyl methyl ether.

- 7. a) What is DEPT in NMR spectroscopy ? Explain its applications.
 - b) Deduce the structure of a compound $C_8H_{10}O$ which gives 1H NMR data as $\delta 3.4$ (3H, singlet), 4.5 (2H, singlet), 7.2 (5H, singlet) (ppm).

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- 8. a) What are cryptands ? Discuss its structure, properties and uses.
 - b) Explain the "guest-host relationship" in molecular recognition.
- 9. a) Explain the following terms in drug developments by giving suitable illustrationsi) Lead compoundii) Molecular receptors.
 - b) Write the steps involved in the synthesis of phenobarbital.
- 10. a) Illustrate "ultra-sonication and microwave as better tools for organic synthesis" using suitable example.
 - b) What is supercritical CO₂? Discuss its advantages.

(5x5= 25 Marks)

SECTION - C

Answer any three questions. Each question carries 10 marks.

- 11. a) How will you distinguish primary, secondary and tertiary amines using IR spectrum?
 - b) Discuss the important features of the mass spectrum of amines by giving suitable examples.
- 12. Write short notes on :
 - a) Proton decoupled 13C NMR.
 - b) Anisotropic effect and chemical shift.
 - c) Shift reagents.
 - d) Attached proton test (APT) spectrum.
- 13. Describe the preparation, properties and applications of any four synthetic receptors in molecular recognition.
- 14. Write short notes on :
 - i) Synthesis of chloramphenicol.
 - ii) Retrosynthetic analysis and disconnection approach.
- 15. Discuss the designing of a green synthesis with suitable examples.

- ---- reaction.

 $(3 \times 10 = 30 \text{ Marks})$

(Pages : 3)

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Third Semester M.Sc. Degree Examination, January 2017 Branch : Chemistry CL/CA/CH 232 : ORGANIC CHEMISTRY – III (2013 Admission Onwards)

Time: 3 Hours

Max. Marks: 75

SECTION - A

Answer **any two** among **(a), (b)** and **(c)** from **each** question. **Each** sub-question carries **2** marks.

- 1. a) How will you distinguish CH_3OCH_3 and C_2H_5OH using IR spectroscopy?
 - b) Compare the stretching frequencies of C C, C = C and C = C by giving reasons.
 - c) What is McLafferty rearrangement in mass spectroscopy?
- 2. a) Acetylenic H's are at a higher field than vinylic H's in PMR spectra give reason.
 - b) What is DEPT in NMR spectroscopy?
 - c) Give the number of signals in the proton spin decoupled 13C spectrum of 3-hexanone, $CH_3CH_2COCH_2CH_2CH_3$.
- 3. a) What are cryptands ? Write an example.
 - b) Explain supramolecular organic nanotubes (ONTs). Give an application.
 - c) What are methane clathrates ? Write two applications.
- 4. a) Give the structure of benzyl penicillin.
 - b) What is Taft equation ? How it is superior to Hammett equation for structure reactivity relationship ?
 - c) Write the steps involved in the synthesis of paracetamol.

B – 4318

- 5. a) What are the characteristics of ionic liquids ?
 - b) What is meant by "reaction mass balance"?
 - c) What is sonication ? Give an example for sonication assisted organic synthesis.
 (2×10= 20 Marks)

-2-

SECTION - B

Answer either (a) or (b) of each question. Each question carries 5 marks.

- 6. a) The dehydration of 1,2-dimethyl cyclohexanol gives three probable alkenes. Explain how IR spectroscopy is used to differentiate the alkenes.
 - b) Write the fragmentation pattern to account the major peaks of each of the following compounds
 - i) $CH_3CH_2COOCH_3$; m/z = 57, 59 and 88
 - ii) $CH_3OCH_2CH_2CH_3$; m/z = 31, 45, 59 and 74.
- 7. a) i) Give reasons why TMS is used as a reference compound in NMR.
 - ii) What are the important characteristics of a solvent used in NMR?
 - b) Deduce the structure of a compound $C_7H_7NO_3$ which gives 1H NMR data as δ 3.9 (3H, singlet), 6.9 (2H, doublet), 8.1 (2H, doublet) (ppm)
- 8. a) Describe briefly "molecular receptors".
 - b) Write short notes on :
 - i) Organic zeolite and
 - ii) Calixarenes.
- 9. a) Explain briefly on retrosynthesis by giving suitable examples.
 - b) Write the steps involved in the synthesis of chloramphenicol.
- 10. a) Write notes on :
 - i) biocatalysts.
 - ii) sustainability in green chemistry.
 - b) Give the synthesis of any two organic compounds using microwave heating as green technology. (5×5= 25 Marks

SECTION - C

Answer any three questions. Each question carries 10 marks.

- 11. Discuss the different types of electronic transitions and transition probabilities. Explain the effect of polarity of solvent on each transition.
- 12. Write short notes on :
 - i) Nuclear Overhauser Effect (NOE).
 - ii) Factors which affect the magnitude of chemical shift.
 - iii) Proton exchange reaction.
 - iv) Coupling constant.
- 13. Describe the different types of driving forces involved in the formation of supramolecular structures with suitable examples.
- 14. Write notes on :
 - i) Modeling studies in drug design
 - ii) Combinatorial organic synthesis.
- 5. What are the twelve basic principles of green chemistry ? Explain any four with suitable examples. $(3 \times 10 = 30 \text{ Marks})$

(Pages : 3)

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Reg. No. :

Name :

Third Semester M.Sc. Degree Examination, January 2018 Branch : Chemistry CH/CL/CA/CM 232 : ORGANIC CHEMISTRY - III (2016 Admission)

Time : 3 Hours

Max. Marks: 75

SECTION - A

Answer **any two** among (**a**), (**b**) and (**c**) from **each** question. **Each** sub-question carries **2** marks.

- 1. a) What is the advantage of chemical ionization technique in MS?
 - b) Why OH absorption for alcohols in IR is very broad?
 - c) Why red shift occurs in enones and compare to ketone in UV-V is spectrum?
- 2. a) Define chemical shift.
 - b) Name three shift reagents.
 - c) Explain the term polarization transfer in NMRI.
- 3. a) Give an example for chichibabin reaction.
 - b) Complete the following reaction.



- c) What are the reagents for Oppeneaur oxidation? Give an example.
- 4. a) Give an example for Globe reaction.
 - b) What is meant by chiral auxiliary?
 - c) How do you protect an amino group?
- 5. a) Differentiate between adsorption and partition chromatography.
 - b) What is centrifugal TLC?
 - c) List out the column used in GC.

(10×2=20 Marks)

b) Write the number of signals and splitting pattern



$$CH_3 - C - CH_3 + CH_2O + CH_3NH_2 \xrightarrow{Base}$$

- b) Discuss Peterson's olefination with suitable example.
- 9. a) What is meant by stereoselective synthesis? Discuss with an example.
 - b) Disconnect the following molecule and suggest suitable method of synthesis of target molecule.





- 10. a) Explain the Craig's technique of liquid-liquid extraction.
 - b) Discuss the application of capillary electrophoresis.

(5×5=25 Marks



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SECTION - C

Answer any three questions. Each question carries 10 marks.

- 11. Illustrate instrumentation and application of mass spectrometry.
- 12. i) Discuss HSQC with suitable example.

ii) An organic molecule of molecular formula $C_7H_6O_2$ having the following spectral IR (KBr) : 3025 (Br), 1690, 1235 cm⁻¹ Mass (m/z): 122 (30%), 105 (100%), 77(80%), ¹H NMR : 7.4 – 8.1(5H, m), 11.8 (1H, s) ¹³C NMR : 128.4, 130.2, 133.83, 172.7 ppm. Assign the structure of the compound.

- 13. Discuss the following reactions with mechanism : i) Clemmenson reduction

 - ii) Stork enamine reaction.
- 14. i) Discuss the electrochemical reduction of Nitro and Carbonyl groups.
 - ii) What is metathesis ? Explain with suitable example.
- 15. Illustrate the instrumentation and working of HPLC.

(3×10=30 Marks)

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(Pages : 3)

D - 3930

Third Semester M.Sc. Degree Examination, January 2018 **Branch : Chemistry** CH/CL/CA 232 - ORGANIC CHEMISTRY - III (2013 Admission)

Time: 3 Hours

Max. Marks : 75

SECTION - A

Answer any two sub-questions among (a - c) from each question. Each sub-question carries 2 marks.

- 1. a) Predict the λ_{max} for the following compound using Woodward Fieser rules :

 - b) Suggest a suitable spectroscopic technique to differentiate between methyl 2-hydroxybenzoate and methyl 4-hydroxybenzoate. Justify.
 - c) What is Mc Lafferty rearrangement in MS ? Give an example.
- 2. a) How will you define a first-order spectrum in NMR ?
 - b) Comment on the nature of signals obtained for CH₃, CH₂ and CH in APT experiments.
 - c) Draw a stick spectrum for ethylbenzene indicating approximate chemical shifts of all protons and splitting patterns for $-CH_2$ and $-CH_3$ protons.
- 3. a) List out the important intermolecular forces involved in molecular recognition.
 - b) What are crown ethers ? Explain the nature of non-covalent forces involved in cation binding by crown ethers.
 - c) Explain the term self-assembly in supramolecular chemistry.

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c) What are enamines ? Write one synthetic application of enamine.

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a) State and explain the terms involved in Hammet equation.

b) What are analgesics and antipyretics ? Give examples with structures.

c) How is the synthesis of the β -lactam ring achieved in penicillin synthesis ?

- 5. a) What is the important of ionic liquids in organic synthesis ?
 - b) Differentiate between yield and atom economy of a reaction.
 - c) Give a schematic diagram of a single mode microwave cavity.

(2×10=20 Marks

SECTION - B

Answer either (a) or (b) of each question. Each question carries 5 marks.

- 6. a) Give a comparative account of EI and CI modes of ionization in mass spectroscopy.
 - b) Draw a schematic diagram of the instrumentation for FTIR and identify the major components and their functions.
- 7. a) Using appropriate examples illustrate AB and AX spin systems in NMR.
 - b) How will you differentiate between n-decane and 4-methylnonane on the basis of IR, UV and MS data ?
- 8. a) Discuss the role of complementary multiple hydrogen-bonding sites in DNA base pairs with appropriate examples.
 - b) Write short notes on a) molecular tweezers b) liquid crystals.
- 9. a) What are the major factors to be considered while choosing a disconnection in retrosynthetic approach ? Discuss.
 - b) Give a short account of the structure activity relationship of drugs.
- 10. a) Write a note on application of sonication in organic synthesis.
 - b) Briefly discuss the concept of a) green solvents b) biocatalysis.

(5×5=25 Marks)

SECTION - C

Answer any three questions. Each question carries 10 marks.

- a) Write a detailed account on factors affecting carbonyl stretching frequency in ketones.
 - b) Explain the following : i) red shift, ii) TOF mass analyser.
- 12. Briefly discuss the applications of NOE, APT, DEPT and INEPT techniques in NMR spectroscopy.
- 13. Write brief notes on a) molecular receptors, b) self-association in nature, c) industrial applications of supramolecular chemistry.
- 14. Give a detailed account of combinatorial organic synthesis.
- 15. Highlight the significance of green reaction media and green processes. (3×10=30 Marks)

eminos 2 Write one synthetic application of enamine.

(Pages : 4)

Reg. No. :

Name :

Third Semester M.Sc. Degree Examination, January 2020

Chemistry/Polymer Chemistry

CH/CL/CM/CA/ PC 232 : ORGANIC CHEMISTRY-III

(Common for Chemistry (2016 Admission Onwards) and Polymer Chemistry (2018 Admission))

Time : 3 Hours

Max. Marks: 75

SECTION - A

(Answer any two among (a), (b) and (c) from each question. Each sub question carries 2 marks)

- 1. (a) Compare the relative red shifts of p-nitroaniline and p-diaminobenzene.
 - (b) Predict the relative IR absorption values (approximate) due to C=O stretch in an aldehyde, ketone and amide.
 - (c) Give any two major peaks and the mode of their formation in the mass spectrum of ethyl benzoate.
- 2. (a) The NMR spectrum of dimethyl formamide at room temperature shows two peaks for its methyl groups. Why?
 - (b) Write the advantages of the 2D NMR technique, COSY.
 - (c) Why are acetylenic hydrogens more up-field than vinylic hydrogens?



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- 3. (a) Give the reagent and conditions for the selective conversion of an ∞ , β -unsaturated ketone to the respective alcohol.
 - (b) Write the mechanism of carbon-carbon bond formation between an alkene and an alkyl halide using palladium catalyst.
 - (c) Explain an application of HI04 in organic synthesis.
- 4. (a) Write the method of conversion of acetaldehyde to acetone using umpolung.
 - (b) Explain the term combinatorial synthesis.
 - (c) What is Mitsunobu reaction?
- 5. (a) Differentiate between "Gradient Elution" and "Isothermal Elution" in chromatogtaphy.
 - (b) What is the principle of capillary zone electrophoresis?
 - (c) Why liquid chromatography is a viable technique for the separation of proteins, nucleosides etc., as compared to gas chromatography?

(2 × 10 = 20 Marks)

SECTION - B

(Answer either (a) or (b) from each question. Each sub question carries 5 marks)

6. (a) (i) By using Woodward Fieser rules calculate the Amax values for the following compounds.





(ii) Which has a lower characteristic stretching frequency, the C-H or C-D bond? explain briefly.



- (b) (i) What are the predicted m/z values (masses) and relative heights of all the molecular ions of 1-bromoethane that would appear on a mass spectrum (excluding peaks produced by ¹³C and ²H)?
 - (ii) Write short notes on metastable ions
- (a) What is anisotropic effect? Explain the paramagnetic anisotropy of alkene, aldehydic and aromatic protons.
 - (b) Predict the number of signals and their chemical shift and spin-spin coupling in each of the following compounds in ¹H NMR spectra.
 - (i) CH_3 - CH_2 -CI
 - (ii) CH_3 -CH(CI)-CH₃
 - (iii) Br-CH₂-CH₂-CH₂-Br
- 8. (a) What is an enamine? How it is prepared? Give two synthetic applications.
 - (b) With suitable examples (two), illustrate the application of Peterson olefination in stereoselective synthesis of alkenes.
- 9. (a) Explain the details of Sharpless asymmetric epoxidation of allylic alcohols.
 - (b) Write short note on
 - (i) Electrochemical kolbe oridation
 - (ii) Olefin metathesis.
- 10. (a) Explain the development of TLC plates. How do you choose the solvents for the development of TLC plates?
 - (b) Discuss the affinity and chiral separations using HPLC.

 $(5 \times 5 = 25 \text{ Marks})$

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SECTION - C

(Answer any three questions. Each question carries 10 marks)

- 11. Describe briefly the major ion production techniques in mass spectrometry.
- 12. (a) Draw the proton decoupled ¹²C-NMR, DEPT-45, 90 and 135 spectra of given compound.



- (b) Write notes on
 - (i) Shift reagents
 - (ii) HMBC 2D NMR spectra.

13. Write notes on the following

- (a) Mannich reaction
- (b) Wolf-Kishner reduction
- (c) Shapiro reaction
- (d) Suzuki coupling
- 14. Discuss the advantages and disadvantages of hydroxyl, thiol, carboxyl, and carbonyl protecting groups used in organic synthesis.
- 15. Explain the applications of Gas chromatography in separation, identification and quantitative analysis of organic compounds

 $(3 \times 10 = 30 \text{ Marks})$





Reg. No. : Name :

Third Semester M.Sc. Degree Examination, February 2021

Chemistry/Polymer Chemistry

CH/CL/CA/CM/PC 232 - ORGANIC CHEMISTRY - III

Common for Chemistry (2016 Admission Onwards) and

Polymer Chemistry (2018 Admission Onwards)

Time : 3 Hours

Max. Marks: 75

SECTION - A

Answer any two among (a), (b) and (c) from each questions. Each sub question carries 2 marks.

- 1. (a) Determine the structure of the compound. Molecular formula C_3H_6O , $\lambda_{max} = 292 \text{ nm and } \varepsilon_{max} = 21$; IR (1) 2720 cm⁻¹(w) and (2) 1738 cm⁻¹(s).
 - (b) A nitrogen containing aromatic compound shows bands at 1550 and 1350 cm⁻¹. Identify the functional group present in it.
 - (c) Indicate which absorption bands in the IR spectrum can be used to distinguish between the following pairs of compounds :
 - (i) (CH₂)₃N and (CH₃)₂CHNH₂,
 - (ii) CH₃CH₂OH and CH₃CO₂H

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- (a) Explain the advantages of TOF mass analysers? 2.
 - (b) What do you meant by DEPT?
 - Give the splitting pattern in the ¹H NMR ^{spectrum} of CH₂=CHBr. (a) What are the different factors affecting the rate of Chichibabin reaction.
 (b) Predict the
- 3.
 - (b) Predict the products of the following reactions :



 H_2 , (R)-BINAP-Ru(II) 100 atm. 40°C (ii) COOBu

- (c) What are the advantages of osmium tetroxide compared to KMnO4 in hydroxylation of alkenes? What are the disadvantages?
- (a) What is chiral pool synthesis? 4.
 - (b) Describe Kolbe oxidation
 - (c) What are synthons? How is it related with synthetic equivalents?
- (a) What is the principle of column chromatography? 5.
 - (b) Describe the application of paper chromatography in identifying different
 - (c) What is capillary electrophoresis?

SECTION - B

Answer (a) or (b) of each question and each question carries 5 marks.

- 6. (a) Discuss briefly about Nuclear Overhauser Effect (NOE)?
 - (b) Explain nitrogen rule. Explain how it is useful in determining the molecular formula.
- 7. (a) What is olefin metathesis? Discuss the synthetic applications.
 - (b) Discuss the mechanism and applications of Mitsunobu reaction.
- 8. (a) Explain with examples :

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- (i) Shapiro reaction and
- (ii) Ritter reaction.
- (b) Discuss Wolf-Kishner reduction and Oppenauer oxidation.
- 9. (a) Explain the principle of gas chromatography. What type of substrates are analysed using GC?
 - (b) Discuss the principle and applications of solvent extraction.
- 10. (a) Discuss about Electronspray and MALDI ion sources in mass spectrometry.
 - (b) Identify the structure of the compound using following spectral details :

MF : $C_8H_{10}O_2$

IR Bands : 3000, 2951, 2936, 1509, 1464, 1233, 1060, 827 cm⁻¹

¹H NMR : δ 3.75s, 6H, δ 6.83, s, 4 H

¹³C NMR : (off resonance splitting in paranthesis) 56(q), 114(d) and 153 (s) ppm

EIM MS : 138 (Base peak) 123, 95, 41

