CHEM 2430 – Organic Chemistry I – Fall 2015

Instructor: Paul Bracher

Quiz #5

Due: Monday, November 30th, 2015 1:10 p.m. (in class)

| Student Name (Printed) | |
|------------------------|--|
| Student Signature | |

Instructions & Scoring

- Please write your answers on the official answer sheet. No answers marked in this booklet will be graded. Submissions submitted electronically will not be graded.
- You may use any resources you wish and collaborate with others.
- Any questions should be posted to the Blackboard discussion board so all students have equal access to the information.
- Your quiz answer sheet may be photocopied.

| Problem | Points Earned | Points Available |
|---------|------------------|---------------------|
| I | | 30 |
| II | | 16 |
| III | | 18 |
| IV | | 18 |
| V | | 18 |
| TOTAL | | 100 |

Quizzes = Practice Exams. Use this one to Prepare for Exam #4.

Problem I. Multiple choice (30 points total; +5 points for a correct answer, +2 points for an answer intentionally left blank, and 0 points for an incorrect answer). For each question, select the best answer of the choices given. Write the answer, legibly, in the space provided on the answer sheet.

(1)

Not counting those corresponding to solvents or reference standards, how many signals appear in the ¹³C NMR spectrum for compound **A**?

Α

- (a) six
- (b) eight
- (c) ten
- (d) twelve
- (e) fourteen

(2)

How many <u>sets</u> of inequivalent protons contribute to the ¹H NMR spectrum of compound **B**? Note that a set can contain as few as one proton, so long as it is magnetically inequivalent from the others.

В

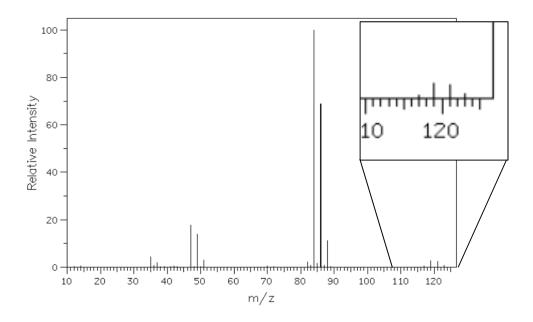
- (a) four
- (b) five
- (c) six
- (d) seven
- (e) eight

(3) _____ Assuming it will be different from the molecular ion, what do you expect to be the base peak for compound **C**?

C

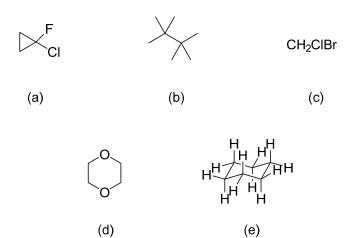
- (a) m/z 12
- (b) m/z 15
- (c) m/z 16
- (d) m/z 57
- (e) m/z 86

(4) _____ Which of the following molecular formulas is consistent with the following mass spectrum?

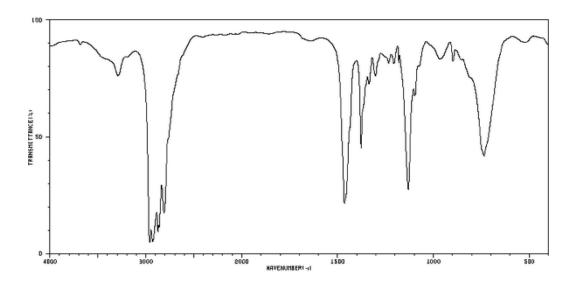


- (a) C₃H₅Br
- (b) CHCIBr
- (c) CHCl₃
- (d) CDCl₃
- (e) C_8H_9N

(5) _____ Which of the following compounds does <u>not</u> have an ¹H NMR spectrum composed of a single peak?



(6) _____ Which of the following compounds is consistent with the IR spectrum shown below?



Problem II. Synthesis (16 points). Outline a synthesis—i.e, a sequence of reactions—to prepare compound **H** from compound **G**. You may use any other reagents you wish. Your final product can be produced as the racemate.

Problem III. (18 points) Roadmap Problem. Provide structures for compounds **J**, **K**, and **M** given the information listed below.

Compound **J** is a hydrocarbon with an 1 H NMR spectrum composed of a single peak. Its electron-impact mass spectrum has a molecular ion peak at m/z 54. When **J** is treated with excess HCl gas, compound **K** is the major product. Compound **K** has a 13 C NMR spectrum with four signals and an 1 H NMR spectrum with three signals: δ 2.4 (quartet), 2.2 (singlet), 1.3 (triplet). Heating **K** with sodamide produces compound **M** as the product, following acidic workup. Its electron-impact mass spectrum also has a molecular ion peak at m/z 54, but its 1 H NMR spectrum has three signals.

Compounds & Reactions Pertinent Spectral Data for Associated Compound Hydrocarbon Electron-impact MS has M⁺ peak of m/z 54 J ¹H NMR spectrum has a single peak excess HCI ¹³C NMR spectrum has 4 signals ¹H NMR spectrum has three signals: roughly δ 2.4 (quartet), Κ 2.2 (singlet), 1.3 (triplet) 1. NaNH₂, heat 2. H₂O Hydrocarbon Electron-impact MS has M⁺ peak of m/z 54 ¹H NMR spectrum has three signals M

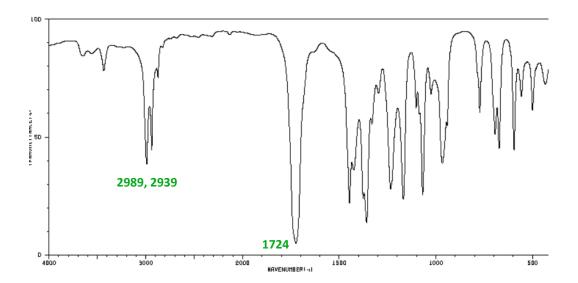
Problem IV. Assignment of an NMR Spectrum (18 points). High-resolution mass spectral analysis of a pure sample of compound **P** reveals it to have a molecular formula of $C_5H_{10}O_3$. The ¹H NMR spectrum of **P** in CDCl₃ has the following signals:

| Chemical Shift (ppm) | Multiplicity | Integration |
|-------------------------|----------------|-------------|
| 11.20 | singlet, broad | 32 |
| 3.71 | triplet | 67 |
| 3.53 | quartet | 64 |
| 2.64 | triplet | 65 |
| 1.21 | triplet | 98 |

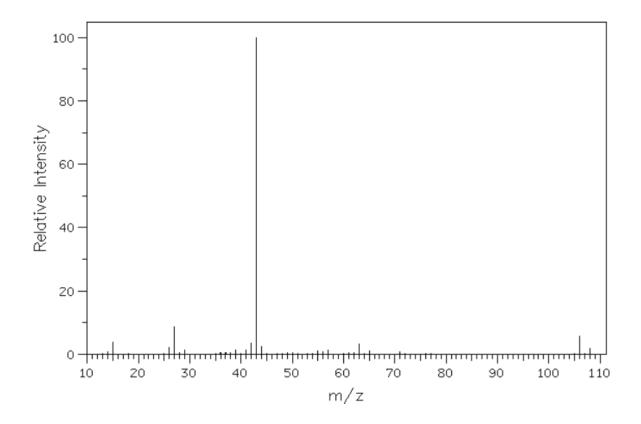
- (i) Draw a Lewis structure for compound **P** consistent with the data provided above.
- (ii) For each chemical shift, draw an arrow pointing to one of the hydrogens that gives rise to that signal.

Problem V. Structure Determination (20 points). Given the spectra shown below for compound **Q**, provide its structure. If you desire partial credit in the event you provide an incorrect answer, show your reasoning by noting important features of the spectra and the portions of the molecule that give rise to these features.

IR Spectrum:

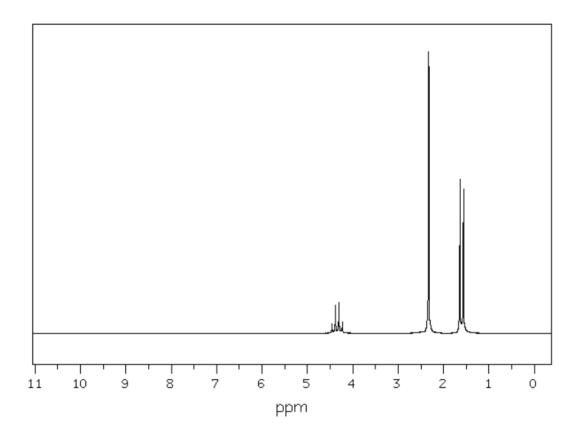


Mass Spectrum:



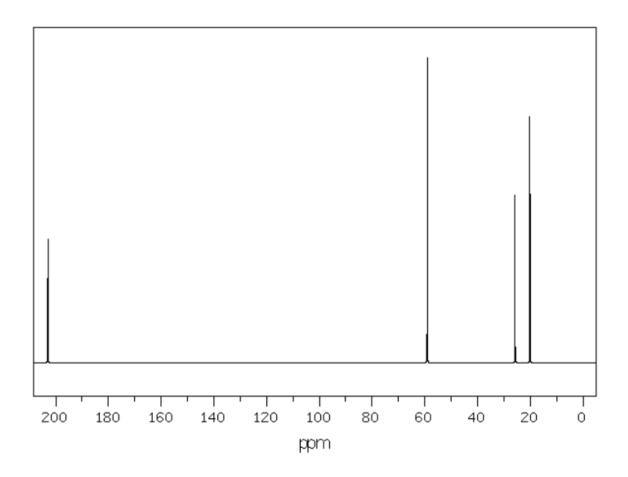
| m/z | Intensity |
|-------|-----------|
| 15.0 | 3.8 |
| 26.0 | 2.2 |
| 27.0 | 8.8 |
| 29.0 | 1.2 |
| 39.0 | 1.2 |
| 41.0 | 1.3 |
| 42.0 | 3.4 |
| 43.0 | 100.0 |
| 44.0 | 2.3 |
| 55.0 | 1.1 |
| 57.0 | 1.3 |
| 63.0 | 3.3 |
| 65.0 | 1.0 |
| 106.0 | 5.8 |
| 108.0 | 1.9 |
| | |

¹H NMR Spectrum:



| Chemical Shift (ppm) | Multiplicity | Integration |
|-------------------------|--------------|-------------|
| 4.32 | quartet | 274 |
| 2.33 | singlet | 819 |
| 1.61 | doublet | 824 |

Proton-decoupled ¹³C NMR Spectrum:



| Chemical Shift (ppm) | Multiplicity | Intensity |
|-------------------------|--------------|-----------|
| 202.95 | singlet | 405 |
| 59.06 | singlet | 1000 |
| 25.72 | singlet | 550 |
| 20.08 | singlet | 805 |