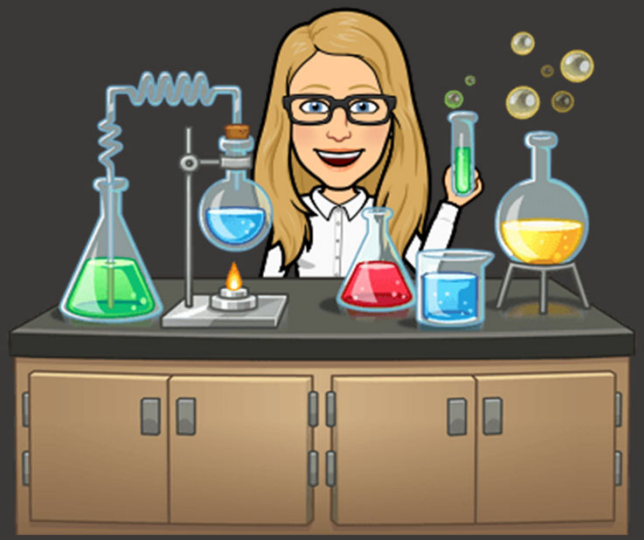
For voting, go to: https://pollev.com/lauriestarke263
or text LAURIESTARKE263 to 37607 to join poll



Dr. Laurie S. Starkey

Cal Poly Pomona

CHM 3140 Organic Chemistry I Announcements 4/16/24

Today's Topic: Exam Review

See Week 12 in Canvas

- **NMR (Ch 15)**
- Chemical Rxns (Ch 6)
- Sn2/Sn1 & E2/E1 (Ch 7)

Organic Chemistry I, CHM 3140, Dr. Laurie
Nuclear Magnetic Resonance (NMR) Spectroscopy, Part 2

^{1}H NMR Problem-Solving Strategies

The goal of solving a ^{1}H NMR spectrum is to determine the structure th
NMR data. Since the NMR provides a lot of data, we must develop a system
determine what pieces are present. Next, we figure out how those pieces fit
our structure to see if it matches the spectral data given.

1) If given an IR spectrum: what functional groups (FG) are present? These a

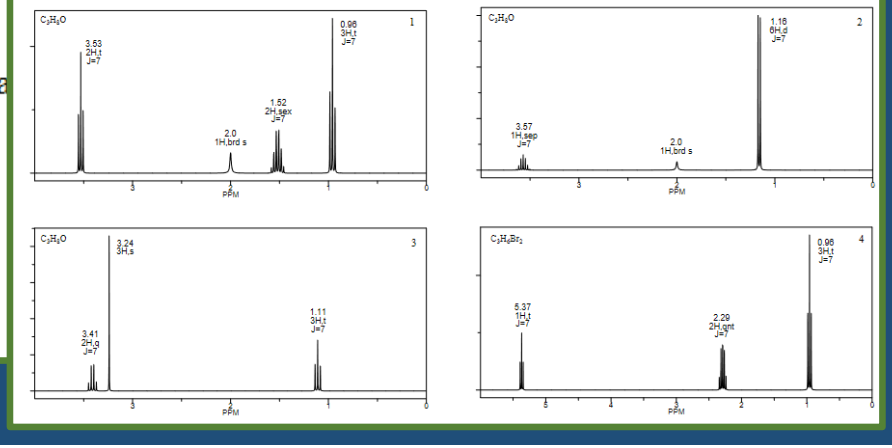
2) If given molecular formula: check for sites/degrees of unsaturation (DU).

If saturated, formula fits $C_nH_{2n+2+\#N}$.

every 2 missing H's = 1 DU

each DU = a π bond or a ring

molecules. Approximate coupling constants are indicated. The multiplicities are s = singlet, d = doublet, t = triplet, q = quartet, qnt = quintet, sex = sextet, se = septet, o = octet, n = nonet, m = multiplet. The degree of unsaturation can help determine the possible number of rings and/or pi bonds. Match each type of hydrogen in the problems with the hydrogen atoms in your structures. Several C NMR problems follow. Propose reasonable structures.



Today's Topic: Exam Review

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Organic Chemistry CHM 3140 Dr. Laurie S. Starkey, Cal Poly Pomona 6-1

Study of Chemical Reactions & Mechanisms - Chapter 6 (Klein)

I) Thermodynamics (6.1, 6.2, 6.3, 6.4) (K_{eq}, ΔG, ΔH, ΔS)
  A) E vs. POR diagrams (6.6)
  B) Estimating ΔH using bond dissociation energies
II) Kinetics and reaction rate variables (6.5)
III) Two-step mechanisms and intermediates (6.6)
  A) carbocation stability (6.8)
  B) carbocation rearrangements (6.11)
IV) Mechanisms and arrow-pushing patterns (6.8, 6.9, 6.10)

Read on your own:
6.12 Reversible & Irreversible Arrows

Moved to Ch. 7:
6.7 Nucleophiles & Electrophiles
(& SkillBuilder 6.2)

Today's Topic: Exam Review

See Week 12 in Canvas

- NMR (Ch 15)
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- **Sn2/Sn1** & E2/E1 **(Ch 7)**

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Dr. Laurie S. Starkey, Organic Chemistry I, CHM 3140

Ch. 7 Summary, Part 1 (Klein 4th Ed.): Alkyl Halides/Substitution Reactions

I. Introduction to Alkyl Halides (7.1, 7.2)
   a. Alkyl, vinyl, aryl halides
   b. Substitution and Elimination reactions

II. Substitution Reactions (R—LG → R—Nu)
   a. Electrophiles (E^+) (6.7)
      i. Contain + or δ^+ sites (e.g., alkyl halides, carbocations)
   b. Nucleophiles (Nu:) (6.7, 7.4)
      i. Contain a source of electrons (e.g., lone pair or pi bond)
      ii. More stable → less reactive, weaker Nu:
      iii. More electron-rich → better Nu:
      iv. Less electronegative → better Nu:
      v. Larger atom → more polarizable, better Nu:
   c. Leaving Groups (7.1, 7.10)
      i. Stable species (weak bases) make good leaving groups (e.g., X^-, TsO^-)
      ii. A good LG makes a favorable substitution reaction ($\Delta G < 0$)
      iii. Make OH a good LG by protonation or tosylation (7.10)

Substitution Reactions

Today's Topic: Exam Review

See Week 12 in Canvas

- NMR (Ch 15)
- Chemical Rxns (Ch 6)
- Sn2/Sn1 & **E2/E1 (Ch 7)**

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Elimination Reactions & Alkenes Summary (Klein

I. Review the pi (π) bond and Nomenclature of alkenes and alkynes (8.3, 9.2)
II. Alkene stability (7.6)
    i) more alkyl groups, more stable
    ii) trans is more stable than cis (except in small rings)
    iii) pi bond unstable at bridgehead carbon (Bredt's Rule)
    iv) alkene is more stable if conjugated with another pi bond (16.2)
III. Alkene synthesis: E2 mechanism (one-step) (7.5, 7.7)
    i) requires strong base (HO^-, RO^-, R_2N^-)
    ii) stereochemistry: *anti*-elimination of β-hydrogen and LG
    iii) regiochemistry: depends on base choice
        i) usually gives the most stable alkene (Zaitsev with NaOH, MeONa, EtONa)
        ii) bulky base gives less substituted alkene (Hofmann with *t*-BuOK)
    iv) often in competition with S_N2 (E2 favored unless primary RX)
IV. Alkene synthesis: E1 mechanism (7.8)
        i) two steps, via carbocation (rearrangement can occur)
        ii) proceeds with loss of stereochemistry (both E and Z alkenes formed)
        iii) regiochemistry: gives the most stable alkene (Zaitsev)
        iv) usually in competition with S_N1 (E1 favored with heat)

Elimination Reactions

Exam III Thursday, 4/18 (Chapters 15, 6, 7)

60-minute written exam

- no Scantron, no lecture after

No notes/calculators/model kits allowed

- Bring pencil(s), eraser

Sample exams on course homepage

- See typical length, format

You must come to your registered section

- 3 pm or 5 pm (Check BroncoDirect)

Extra office hour/review session (lsstarkey OH Zoom)

- Wednesday 4/17, 9-10 pm

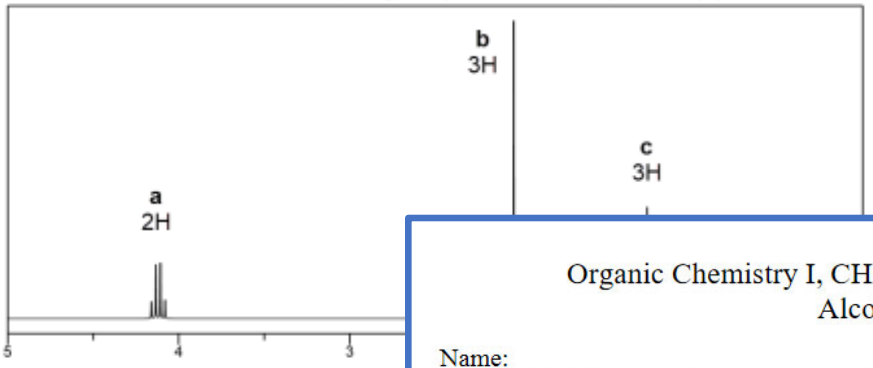
Exam III Free Red Ink:
NMR, Sn1/Sn2 Mech./Dehydration

Don't wait until Thursday night! Set a reminder!

CHM 3140 Organic Chemistry I – Dr. Laurie S. Starkey – NMR Problem Set

Name:_____ Section (day/time):_____

Each of the following ^{1}H NMR spectra comes from a compound with the molecular formula **$C_4H_8O_2$**. Propose a structure for each spectrum and label each proton on the structure (a/b/c..) to match the corresponding signal. Calculation of sites of unsaturation is helpful and careful examination of chemical shifts, integration and splitti
to estimate the chemical shifts (using the provided tables) to verify your answer. **Show you**



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Dr. L. S. Starkey, Organic Chemistry I, CHM 3140, **S_N2 vs. S_N1 Homework**

Name:_____

In the reaction of the tosylate shown and sodium cyanide, both S_N2 and S_N1 mechanisms are possible.

For each reaction: a) predict the major product(s) expected. (stereochemistry?)
b) provide a complete mechanism. (watch details: lone prs, formal charges, arrows)
c) provide an E vs. POR diagram. (give structures for the transition states)

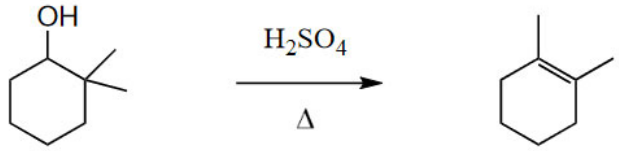
Complete	Bond-line
	ructure or $TsO^{\ominus}$ osylate LG) (see Klein 7.10)

Organic Chemistry I, CHM 3140, Dr. Laurie S. Starkey, Cal Poly Pomona

Alcohol Dehydration Homework

Name:_____ Section: _____ (day/time)

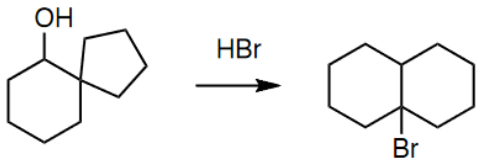
A) Provide a complete mechanism for the following dehyration reaction (pay close attention to details, including lone pairs, formal charges and the use of curved arrows).



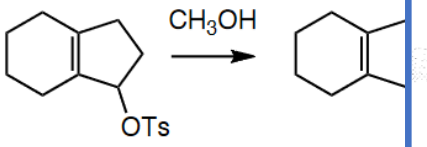
Extra Practice/Exercises on Homepage

CHM 314 Final - Practice Problems (provide complete mechanisms)

Sn1/Carbocation Practice Mechanisms



hint: carbocation rearrangement involves a ring expansion!

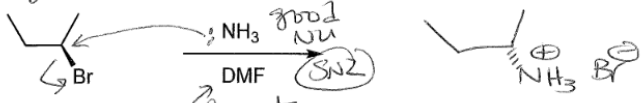


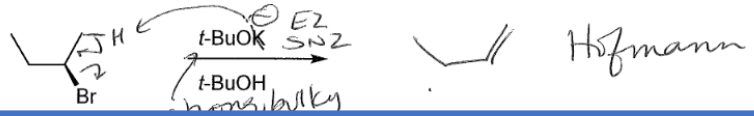
$HO^{\ominus}/RO^{\ominus}$ = strong base (E2 possible)

E2 vs. S_N2: Predict the major product(s) expected for each of the following reactions. Remember to indicate stereochemistry, when appropriate. If no reaction is expected, write NR.

7-18

a) CH_3OTs (S_N2) $\xrightarrow[CH_3OH]{CH_3ONa}$ CH_3OCH_3 (methyl LG)

b) 

c) 

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Comparison of S_N1 and S_N2 Mechanisms

Consider a substitution reaction: RX (Alkyl Halide Electrophile (E^+)) + Nu: (Nucleophile) $\xrightarrow{S_N1 \text{ or } S_N2}$ RNu + X^- (Leaving Group (LG))

S_N1

Rate = k[RX]

no reaction on 1° RX

unimolecular

t-BuBr = fastest

MeOH Nu: H_2O Nu:

carbocation

solvolysis

3° RX

tic solvent

both S_N1 & S_N2

good LG

a bond breaks in rate-determining step

no reaction on vinyl RX

2° RX

S_N2

Rate = k[RX][Nu:]

bimolecular

backside attack

inversion of stereochemistry

MeI = fastest

sterics

no reaction on 3° RX

unhindered E^+

HO^- Nu:

NaOMe Nu:

strong Nu:

only one transition state

1° RX

a bond forms in rate-determining step

aprotic solvent

ollowing items as being related to S_N1, S_N2, or both.

sterics

aprotic solvent

unimolecular

H_2O Nu:

solvolysis

no reaction on vinyl RX

HO^- Nu:

Rate = k[RX]

weak Nu:

strong Nu:

Rate = k[RX][Nu:]

t-BuBr = fastest

no reaction on 3° RX

Using text problems for Self-Assessment

To earn homework credit for Chapters 6, 7-1, 7-2 work on **SkillBuilders** and/or **EOC problems**!

→ Can be hand-written and/or done in WileyPLUS.

→ Submit each to Gradescope by Thursday night.