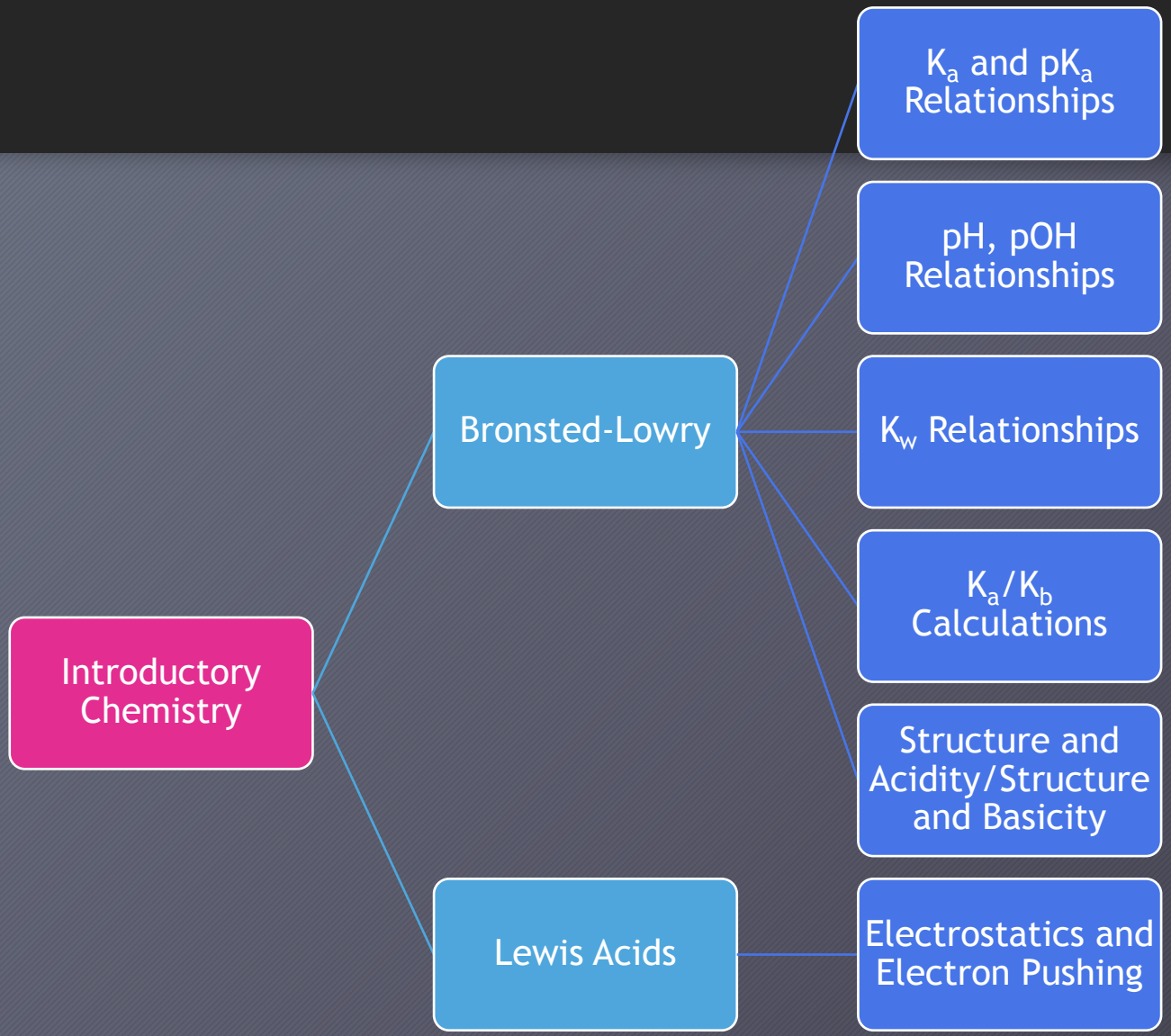
Acid-Base Chemistry: Longitudinal Study Across the Chemistry Curriculum

Charlie Cox, Ph.D.
Associate Professor of the Practice
Duke University

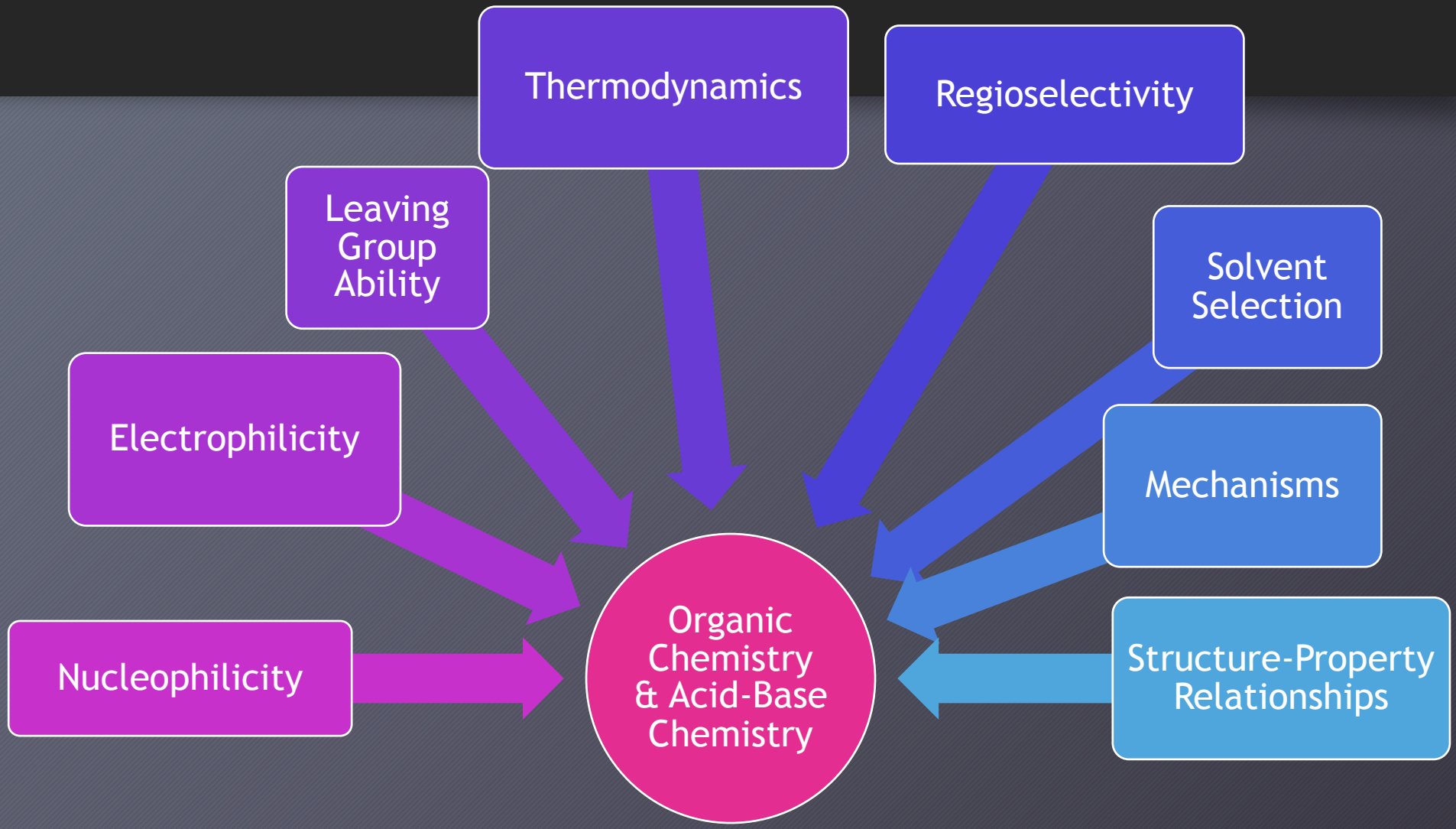
Outline

- Motivation for the Project
- Survey Design
- Basic structure relationships with acid-base chemistry and organic molecules.
- Applications of acid-base chemistry with the Aldol Condensation.

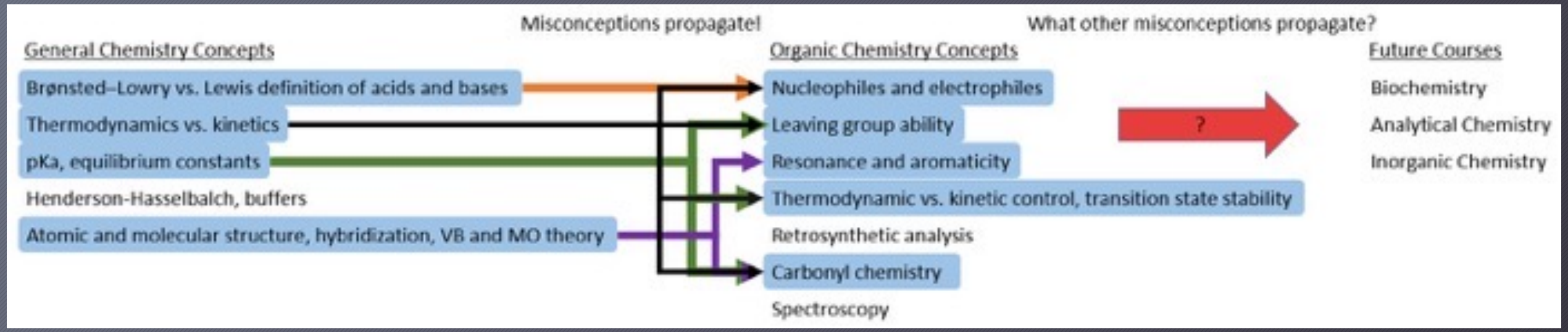
Acid-Base Chemistry and the Chemistry Curriculum



Acid-Base Chemistry and the Chemistry Curriculum



Longitudinal Relationships



Existing Literature

- Sizable research has focused upon acid-base chemistry research in general chemistry.
- McClary focused upon mental models for acids and bases implemented by organic chemistry students.
- Cartrette and Mayo focused upon how students relate acids and bases to organic structure.
-

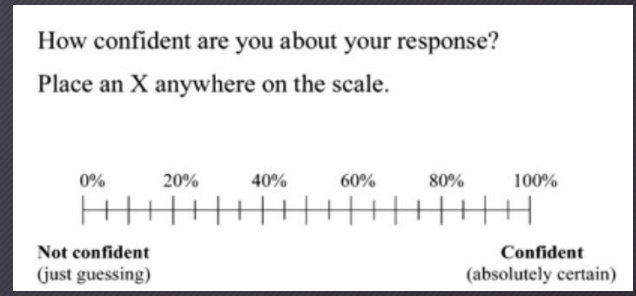
Key Research Questions for the Project

RQ1: How does students' understanding of acid-base chemistry translate to their organic structure-property relationships?

RQ2: How well can students apply their understanding of acid-base chemistry to organic reactivity?

Research Methods

- Construct a survey probing students' ability to apply concepts related to organic structure and reactivity. KR-20 in organic 1 (0.65).
- Design a parallel study for organic chemistry II to determine how students' understanding improves longitudinally.
- Conduct research interviews to further probe student rationale and develop a complete framework outlining student interventions.
- Three overarching questions designed to probe concepts of reaction mechanisms, leaving groups, resonance, hybridization, and carbonyl reactions. Each question contained a multiple-choice/ranking portion, an explanation portion, and the following question asking students to rank their confidence



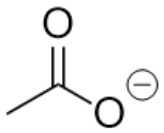
Organic Chemistry I Study

Leaving Group Ability

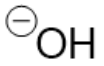
Organic Chemistry & Acid-Base Chemistry

Q1.
The following questions refer to the 3 molecules shown below.

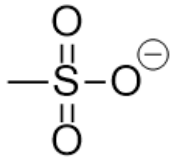
A



B



C



1a.
Rank the above molecules in order of leaving group ability with 1 being the best leaving group and 3 being the worst leaving group.

Molecule A
Molecule B
Molecule C

1b.
Please explain your ranking of the molecules. A 2-3 sentence explanation will suffice.

1c.
How confident are you in your answers to the above questions? 0 = not confident at all, 5 = completely confident

0 1 2 3 4 5

Confidence Level

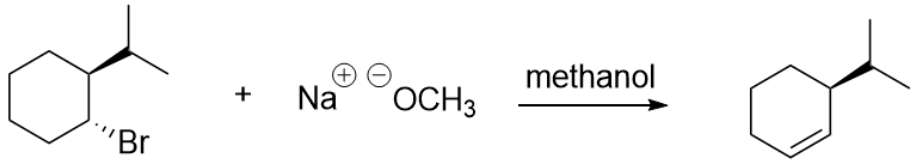
Organic Chemistry I Survey + Organic Chemistry II Survey

Organic Chemistry & Acid-Base Chemistry

Mechanisms

Q2.1

The following questions refer to the reaction shown below.



2a.

Identify the role of methoxide in the given reaction above.

A. Brønsted Acid
B. Brønsted Base
C. Electrophile
D. Nucleophile

2b.

The product of this reaction is formed via which mechanism?

A. E1
B. E2
C. SN1
D. SN2

2c.

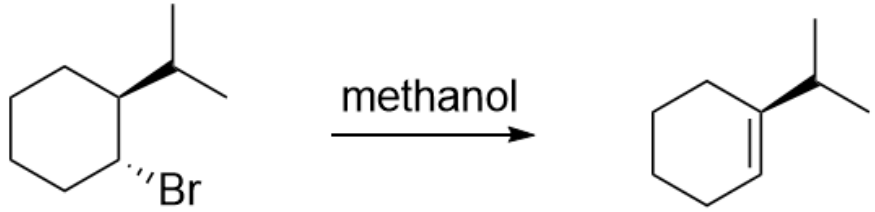
Why does this reaction proceed by the mechanism you selected in part 2b? A 2-3 sentence explanation will suffice.

Organic Chemistry I Study

Organic Chemistry & Acid-Base Chemistry

Mechanisms

Consider now the reaction in the new figure shown below.



2d.
Why does a different product form compared to the reaction shown in the initial figure (Q2.1)? A 2-3 sentence explanation will suffice.

2e.
How confident are you in your answers to all of the above questions? 0 = not confident at all, 5 = completely confident

0 1 2 3 4 5

Confidence Level

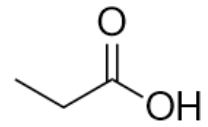
Organic Chemistry I Survey + Organic Chemistry II Survey

Organic Chemistry & Acid-Base Chemistry

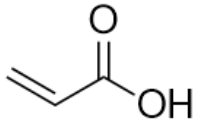
Structure-Property Relationships

The following questions refer to the 3 molecules shown below.

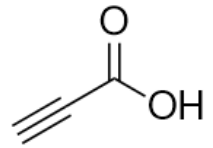
A



B



C



3a.
Rank the above molecules in order of acidity with 1 being most acidic and 3 being least acidic

Molecule A
Molecule B
Molecule C

3b.
Please explain your ranking of the molecules. A 2-3 sentence explanation will suffice.

3c.
How confident are you in your answers to 3a and 3b? 0 = not confident at all, 5 = completely confident

0 1 2 3 4 5

Confidence Level

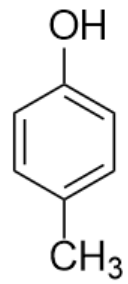
Organic Chemistry II Study

Organic Chemistry & Acid-Base Chemistry

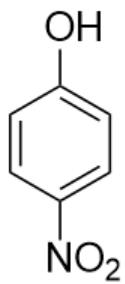
Structure-Property Relationships

The following questions refer to the 3 molecules shown below.

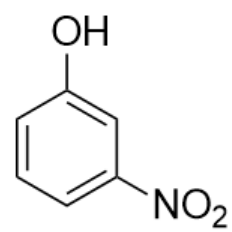
A



B



C



4a.
Rank the above molecules in order of acidity with 1 being most acidic and 3 being least acidic.

Molecule A
Molecule B
Molecule C

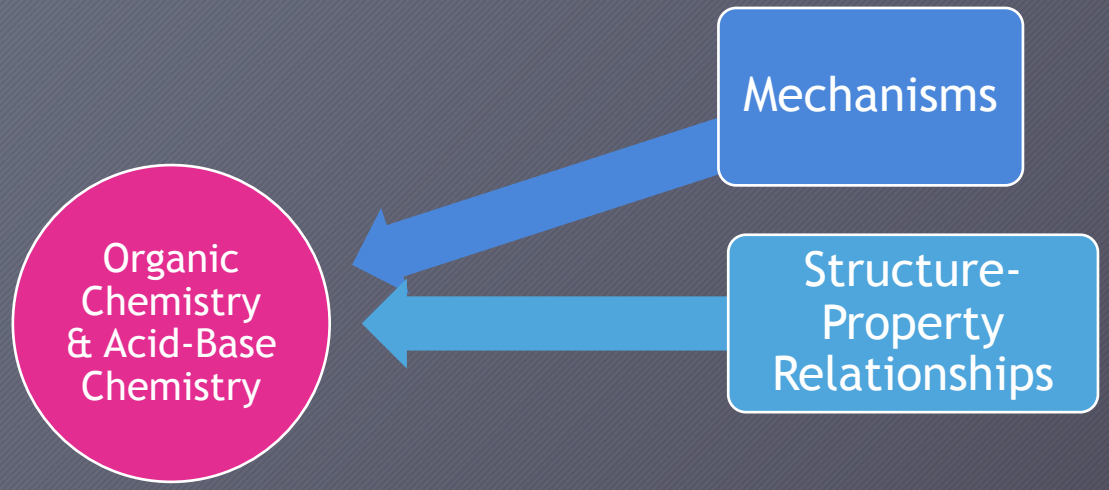
4b.
Please explain your ranking of the molecules. A 2-3 sentence explanation will suffice.

4c.
How confident are you in your answers to 4a and 4b? 0 = not confident at all, 5 = completely confident

0 1 2 3 4 5

Confidence Level

Organic Chemistry I Study



The following questions refer to the 3 molecules listed below.

A) AlH_3

B) NH_3

C) BH_3

D) H^-

4a.
Classify each compound as a Brønsted base, Brønsted acid, Lewis base, and/or Lewis acid. Choose all that apply.

Molecule A	Bronsted Base	Bronsted Acid	Lewis Base	Lewis Acid
Molecule B	Bronsted Base	Bronsted Acid	Lewis Base	Lewis Acid
Molecule C	Bronsted Base	Bronsted Acid	Lewis Base	Lewis Acid
Molecule D	Bronsted Base	Bronsted Acid	Lewis Base	Lewis Acid

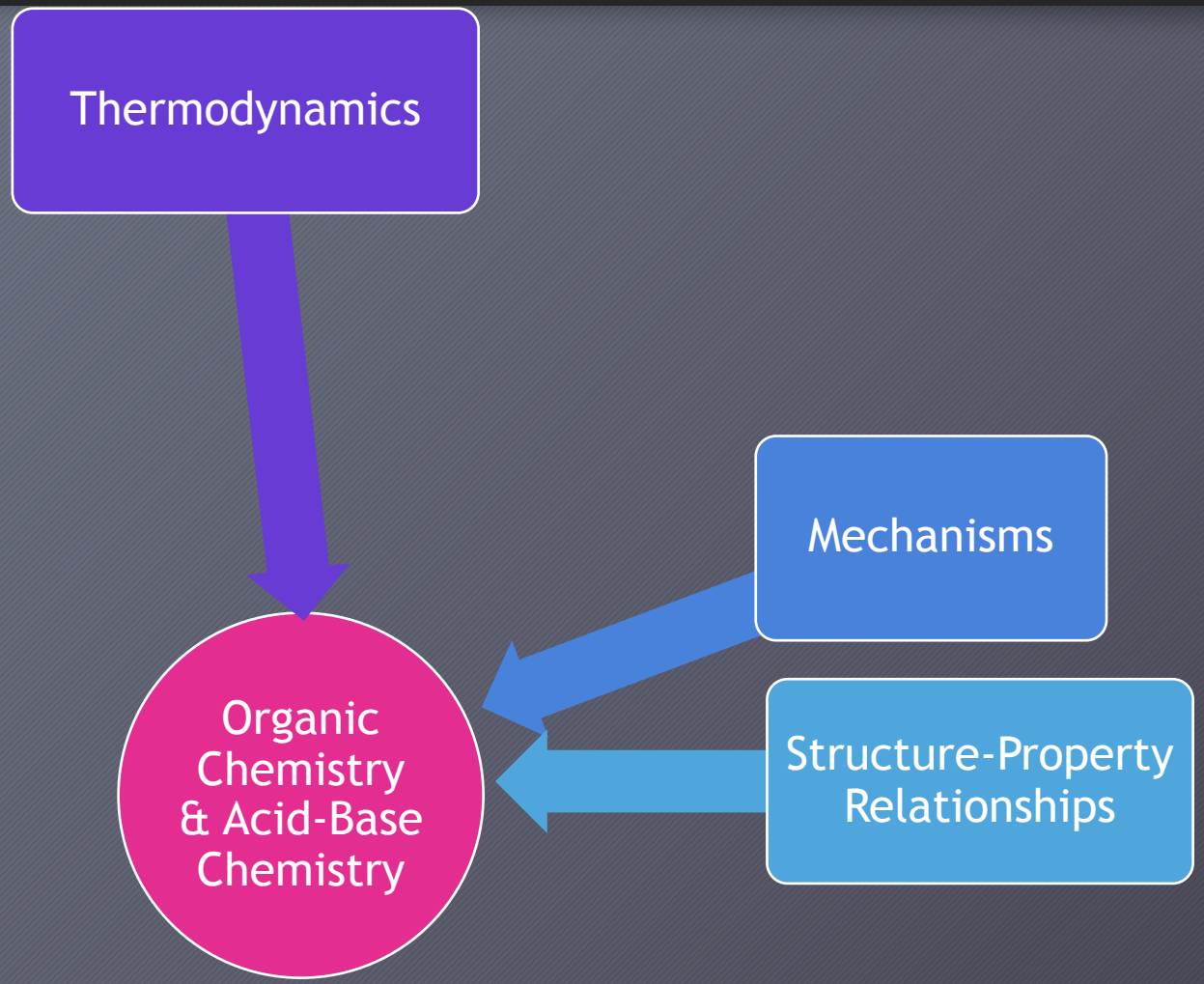
4b.
Please explain your classifications of the compounds above. A 2-3 sentence explanation will suffice.

4c.
How confident are you in your answers to 4a and 4b? 0 = not confident at all, 5 = completely confident

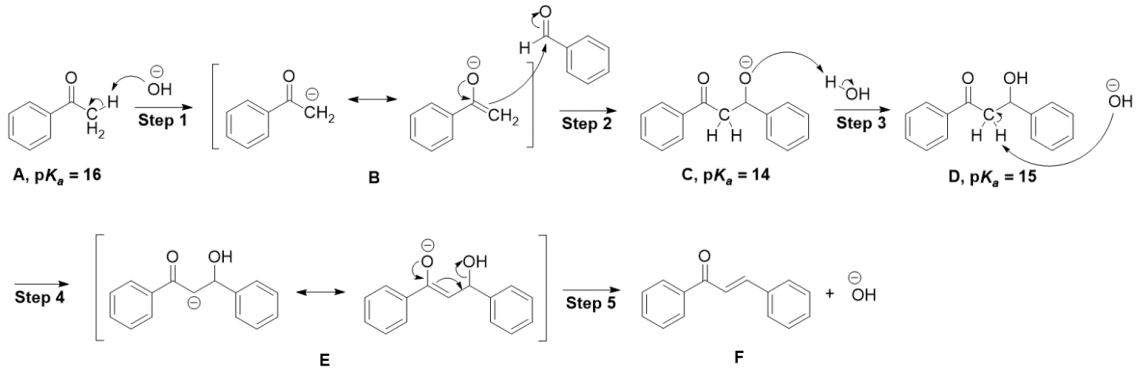
0 1 2 3 4 5

Confidence Level

Organic Chemistry I Survey



The following questions refer to the mechanism shown above. The steps of the reaction are labeled under the reaction arrows. The compounds are labeled A-F and relevant pKa values are provided. Please assume the pKa of water is 14.



5a. For Step 1, which side of the equilibrium will be favored?
Products A
Reactants B
Equally favored

5b. For Step 3, which side of the equilibrium will be favored?
Reactants C
Products D
Equally favored

5c. For Step 4, which side of the equilibrium will be favored?
Reactants D
Products E
Equally favored

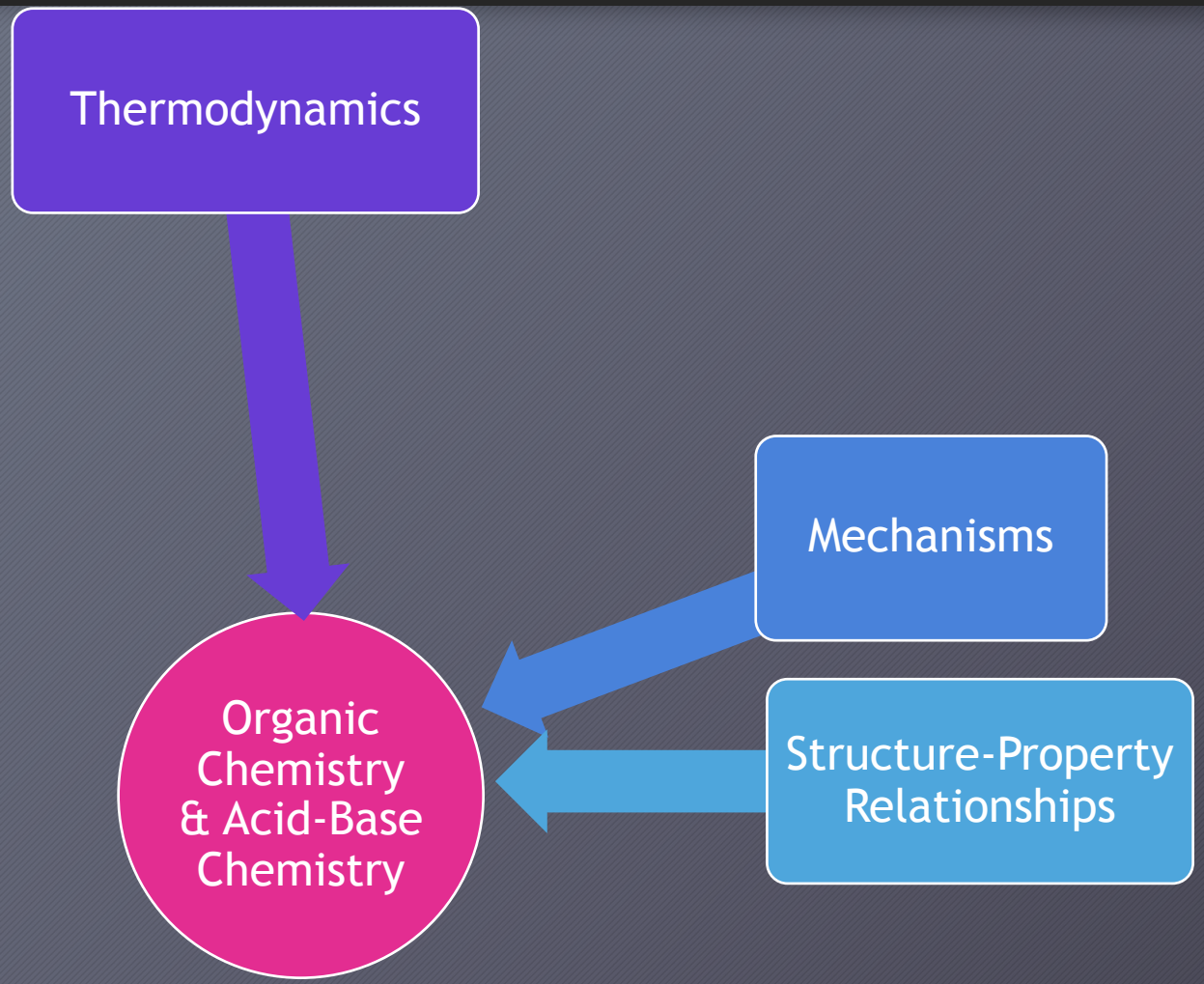
5d.
Please justify your answers to parts a) - c), both in terms of the provided pKa values and the structures of the relevant compounds. A 2-3 sentence explanation will suffice.

5e.
How confident are you in your answers to 5a - 5d? 0 = not confident at all, 5 = completely confident

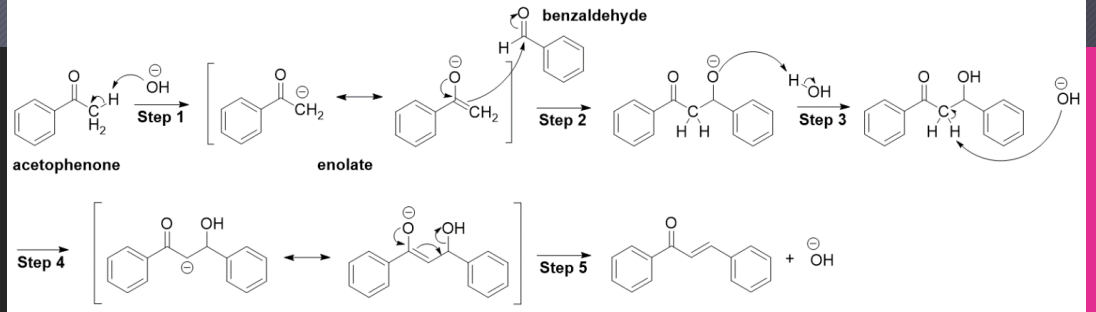
0 1 2 3 4 5

Confidence Level

Organic Chemistry II Survey



The following questions refer to the mechanism shown below. The steps of the reaction are labeled with numbers under the reaction arrows.



5a.
What is the role of hydroxide in step 1?

- Brønsted Acid
- Brønsted Base
- Electrophile
- Nucleophile

5b.
What is the role of acetophenone in step 1?

- Brønsted Acid
- Brønsted Base
- Electrophile
- Nucleophile

5c.
What is the role of the enolate in step 2?

- Brønsted Acid
- Brønsted Base
- Electrophile
- Nucleophile

5d.
What is the role of benzaldehyde in step 2?

- Brønsted Acid
- Brønsted Base
- Electrophile
- Nucleophile

5e.
Which step of this reaction is the least thermodynamically favorable?

Organic Chemistry I Study

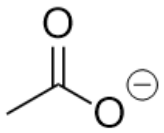
Percent Correct = 81% (9/13)

Explanation = 31% (4/13)

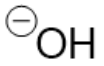
Confidence = 2.75

Q1.
The following questions refer to the 3 molecules shown below.

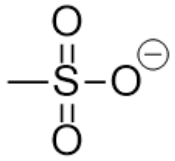
A



B



C



1a.
Rank the above molecules in order of leaving group ability with 1 being the best leaving group and 3 being the worst leaving group.

Molecule A
Molecule B
Molecule C

1b.
Please explain your ranking of the molecules. A 2-3 sentence explanation will suffice.

1c.
How confident are you in your answers to the above questions? 0 = not confident at all, 5 = completely confident

0 1 2 3 4 5

Confidence Level

Key Alternate Conceptions

Students who correctly identified the correct trend, but incorrectly explained why used an incorrect model. Generally this was harder to classify because the students demonstrated a weaker apply to a specific model.

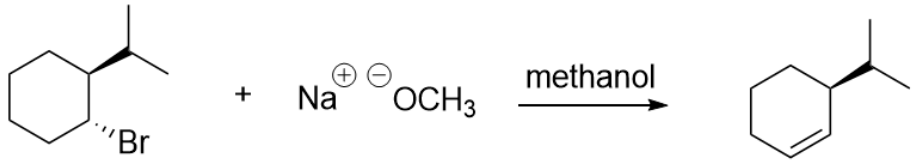
> Based on periodic trends, the O attached to the S is the most acidic due to the size of S.
>
> Sulfur can handle the negative charge better than oxygen.
>
> Weaker bases make the best leaving groups. I know that OH is a strong base, so it would be the worst leaving group. It makes sense for the best to be C because it attaches to Sulfur, which makes the base weaker through polarization.

Organic Chemistry I Study

All students successfully identified the mechanism as E2.

However, only 69% were able to classify the NaOMe as a strong base – in lieu of nucleophile.

Q2.1
The following questions refer to the reaction shown below.



2a.
Identify the role of methoxide in the given reaction above.

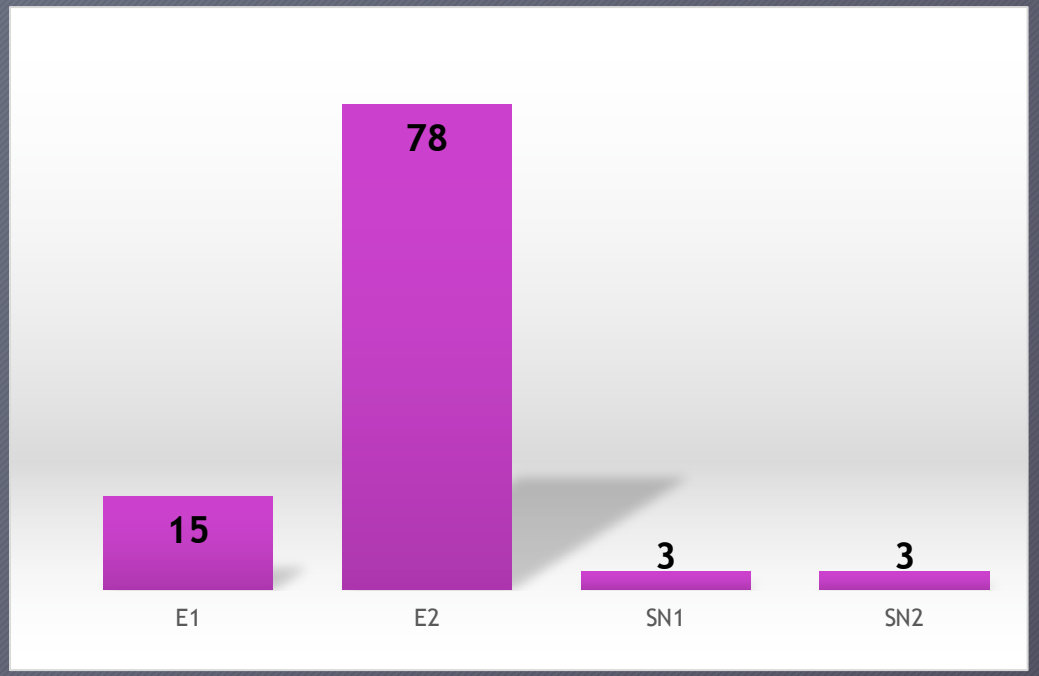
A. Brønsted Acid
B. Brønsted Base
C. Electrophile
D. Nucleophile

2b.
The product of this reaction is formed via which mechanism?

A. E1
B. E2
C. SN1
D. SN2

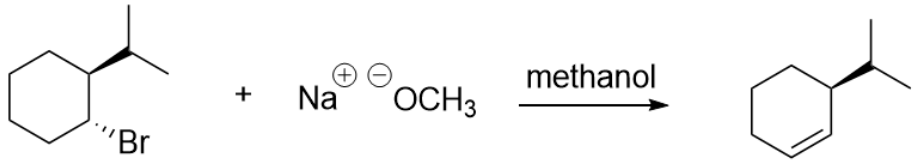
2c.
Why does this reaction proceed by the mechanism you selected in part 2b? A 2-3 sentence explanation will suffice.

Organic Chemistry II Study



Only 78% correctly identified the pathway.
Only 74% correctly labeled methoxide as a base.

Q2.1
The following questions refer to the reaction shown below.



2a.
Identify the role of methoxide in the given reaction above.

A. Brønsted Acid
B. Brønsted Base
C. Electrophile
D. Nucleophile

2b.
The product of this reaction is formed via which mechanism?

A. E1
B. E2
C. SN1
D. SN2

2c.
Why does this reaction proceed by the mechanism you selected in part 2b? A 2-3 sentence explanation will suffice.

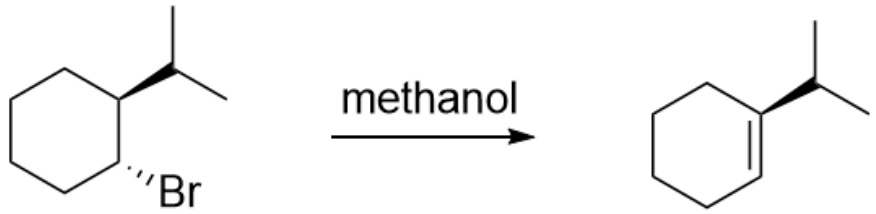
Organic Chemistry I Study

46% recognized that a change in the mechanism from E2 to E1 must be occurring.

The first product was Hofmann while this one is Zaitsev. They are both products of the reaction, it just depends on which beta carbon the double bond is formed on.

The weak base is not as sterically hindered, so it can attack a syn periplanar H on the more substituted carbon.

Consider now the reaction in the new figure shown below.



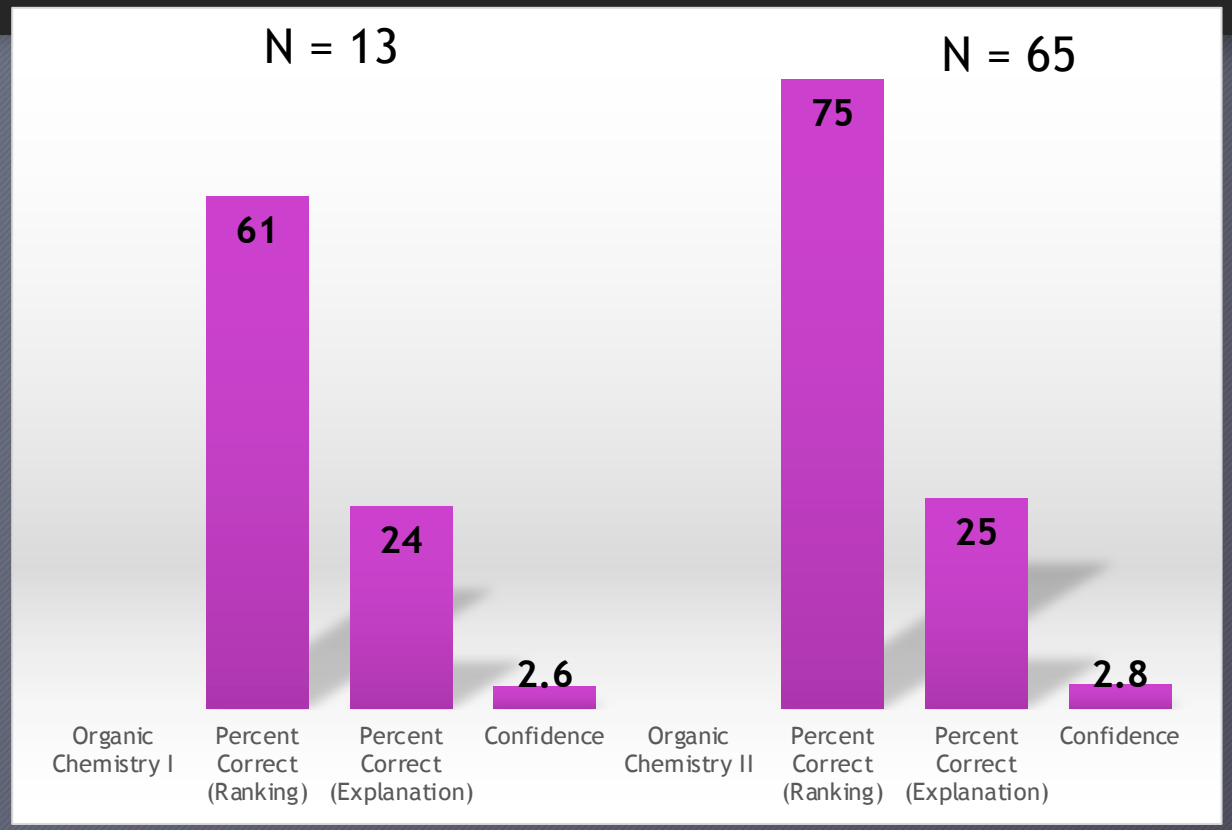
2d.
Why does a different product form compared to the reaction shown in the initial figure (Q2.1)? A 2-3 sentence explanation will suffice.

2e.
How confident are you in your answers to all of the above questions? 0 = not confident at all, 5 = completely confident

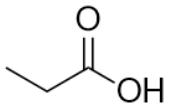
0 1 2 3 4 5

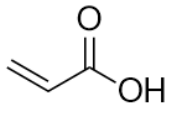
Confidence Level

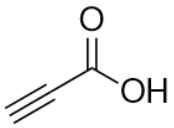
Organic Chemistry I/II Study



The following questions refer to the 3 molecules shown below.

A 

B 

C 

3a.
Rank the above molecules in order of acidity with 1 being most acidic and 3 being least acidic

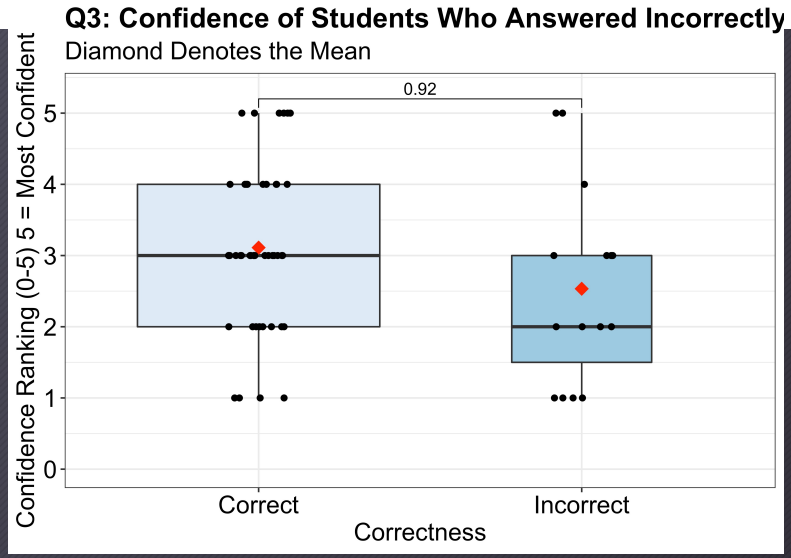
Molecule A
Molecule B
Molecule C

3b.
Please explain your ranking of the molecules. A 2-3 sentence explanation will suffice.

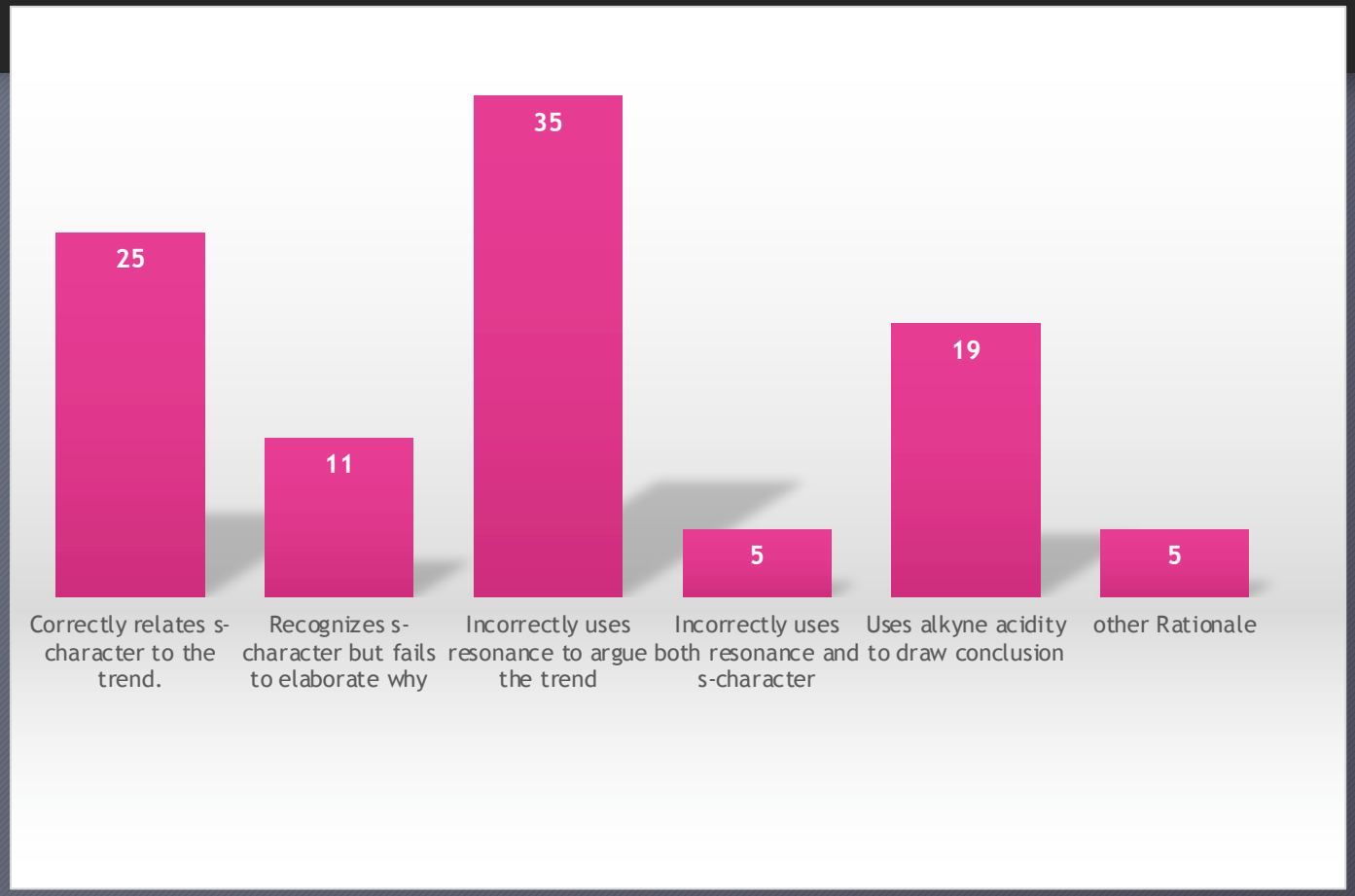
3c.
How confident are you in your answers to 3a and 3b? 0 = not confident at all, 5 = completely confident

0 1 2 3 4 5

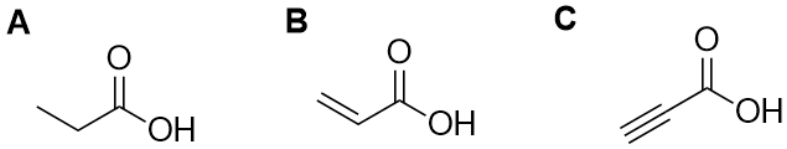
Confidence Level



Organic Chemistry I/II Study



The following questions refer to the 3 molecules shown below.

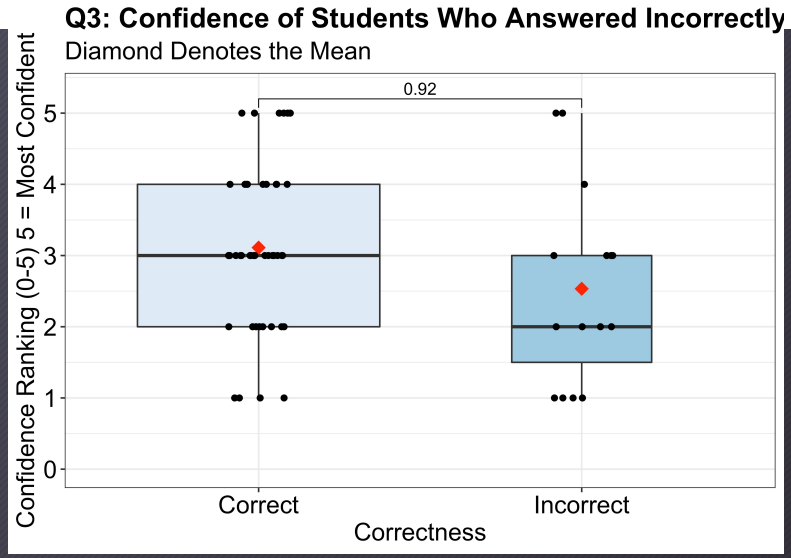


3a.
Rank the above molecules in order of acidity with 1 being most acidic and 3 being least acidic

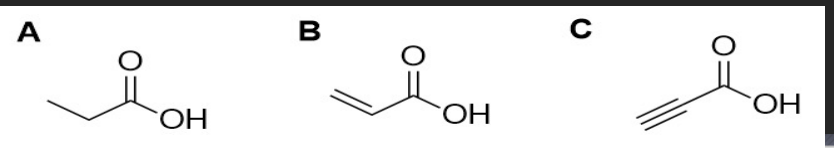
Molecule A
Molecule B
Molecule C

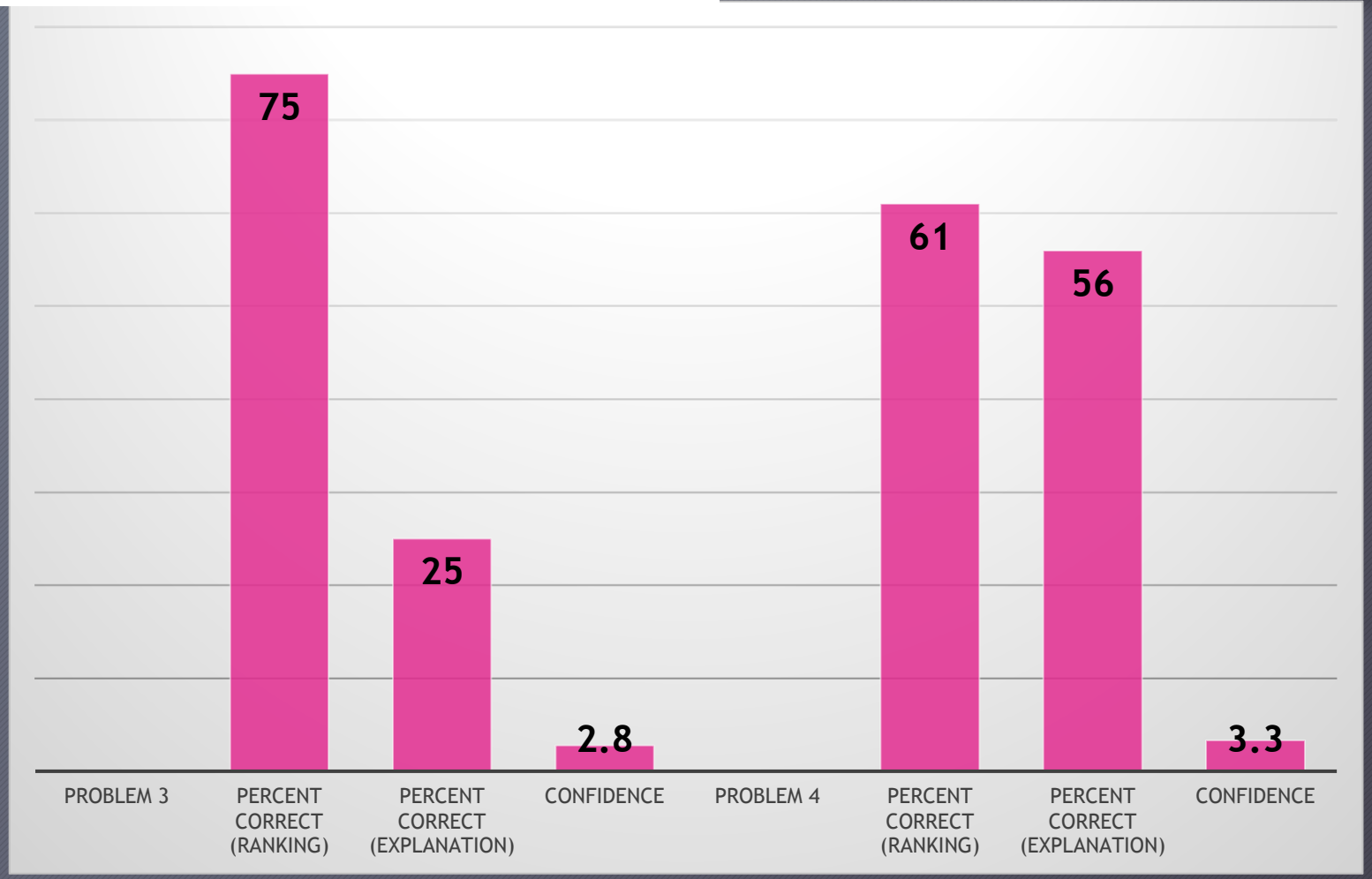
3b.
Please explain your ranking of the molecules. A 2-3 sentence explanation will suffice.

3c.
How confident are you in your answers to 3a and 3b? 0 = not confident at all, 5 = completely confident

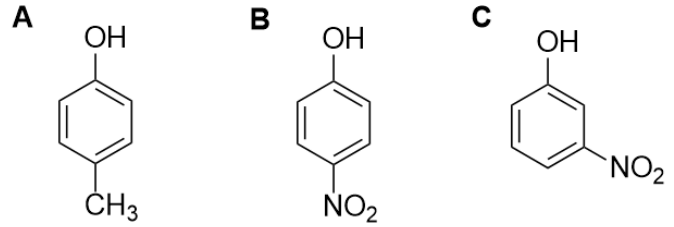


Organic Chemistry II Study





The following questions refer to the 3 molecules shown below.

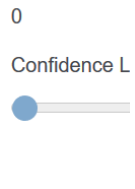


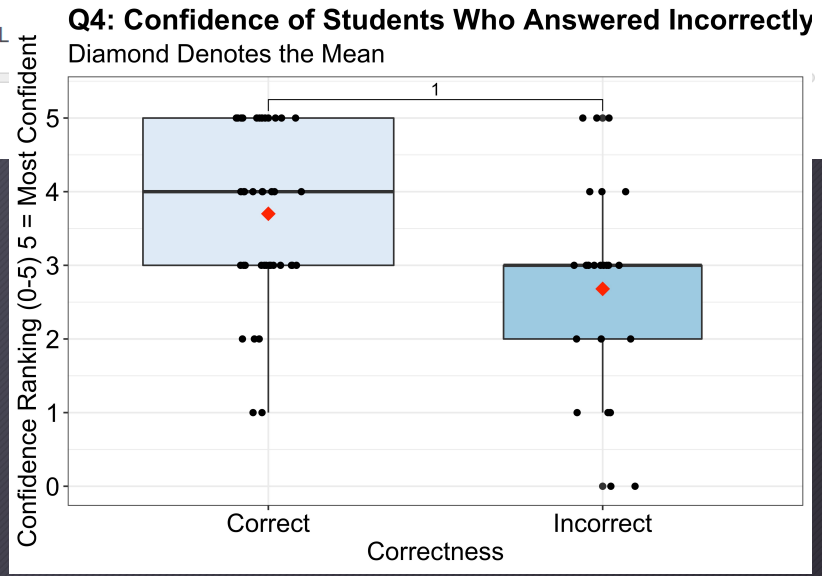
4a.
Rank the above molecules in order of acidity with 1 being most acidic and 3 being least acidic.

Molecule A
Molecule B
Molecule C

4b.
Please explain your ranking of the molecules. A 2-3 sentence explanation will suffice.

4c.
How confident are you in your answers to 4a and 4b? 0 = not confident at all, 5 = completely confident





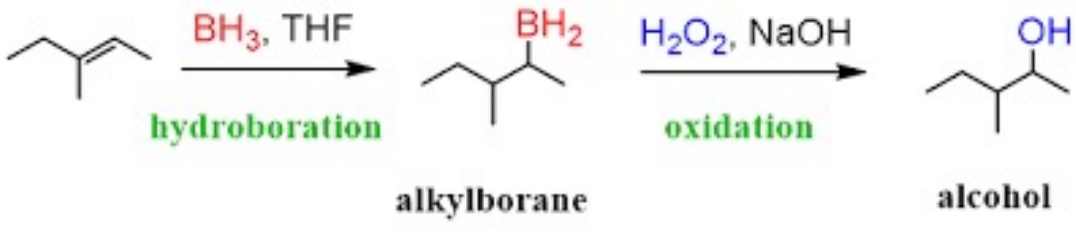
Misconceptions from the Explanations

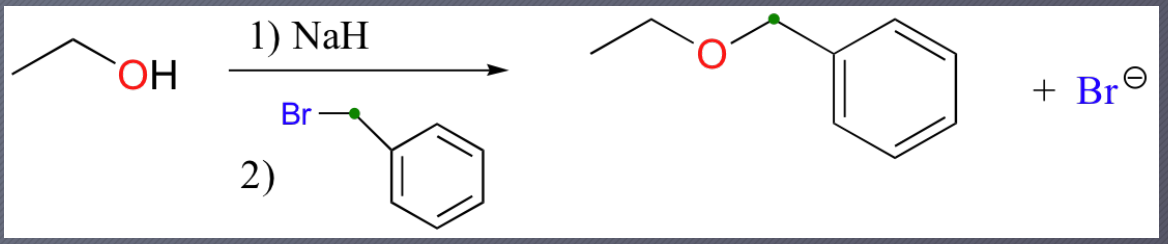
- 14/65 correctly identified para EWG as most acidic, but then believed p-EDG > m-EWG
- 5/65 identified m-EWG as most acidic because it's "closer" to the acidic proton
- Example ideal answer from a student: "B has an EWG in the para position, meaning the electrons can be resonance delocalized into this group. C has an EWG in the meta position, which can inductively stabilize the electrons. A has an EDG, which will destabilize the CB."

Cross Comparison Q3 and Q4

- 33/65 got both questions correct
- 20 people who got Q3 correct missed Q4
- Those who got both correct had a slightly lower average confidence than the average confidence of someone with a correct answer for just Q3 and Q4 respectively. The differences in confidence were not statistically significant using a 95% level of confidence.

Organic Chemistry I Study





Confidence = 1.84

Percent Answering all Correct = 8%

The following questions refer to the 3 molecules listed below.

A) AlH_3 54%

B) NH_3 38%

C) BH_3 31%

D) H^- 24%

4a.
Classify each compound as a Brønsted base, Brønsted acid, Lewis base, and/or Lewis acid. Choose all that apply.

Molecule A	Bronsted Base	Bronsted Acid	Lewis Base	Lewis Acid
Molecule B	Bronsted Base	Bronsted Acid	Lewis Base	Lewis Acid
Molecule C	Bronsted Base	Bronsted Acid	Lewis Base	Lewis Acid
Molecule D	Bronsted Base	Bronsted Acid	Lewis Base	Lewis Acid

4b.
Please explain your classifications of the compounds above. A 2-3 sentence explanation will suffice.

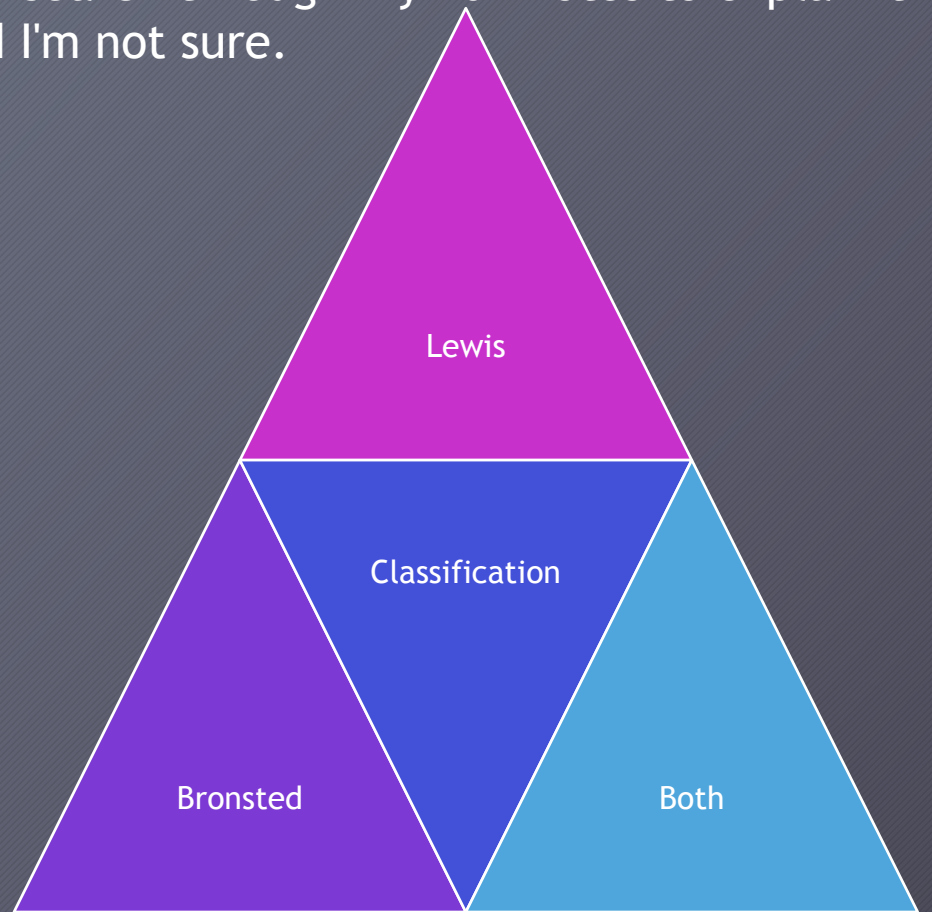
4c.
How confident are you in your answers to 4a and 4b? 0 = not confident at all, 5 = completely confident

0 1 2 3 4 5

Confidence Level

Organic Chemistry I Study

I'd have to see the compounds in the context of a reaction, or search through my 101 notes to explain this. But offhand I'm not sure.



The following questions refer to the 3 molecules listed below.

A) AlH_3 54%

B) NH_3 38%

C) BH_3 31%

D) H^- 24%

4a.
Classify each compound as a Brønsted base, Brønsted acid, Lewis base, and/or Lewis acid. Choose all that apply.

Molecule A	Bronsted Base	Bronsted Acid	Lewis Base	Lewis Acid
Molecule B	Bronsted Base	Bronsted Acid	Lewis Base	Lewis Acid
Molecule C	Bronsted Base	Bronsted Acid	Lewis Base	Lewis Acid
Molecule D	Bronsted Base	Bronsted Acid	Lewis Base	Lewis Acid

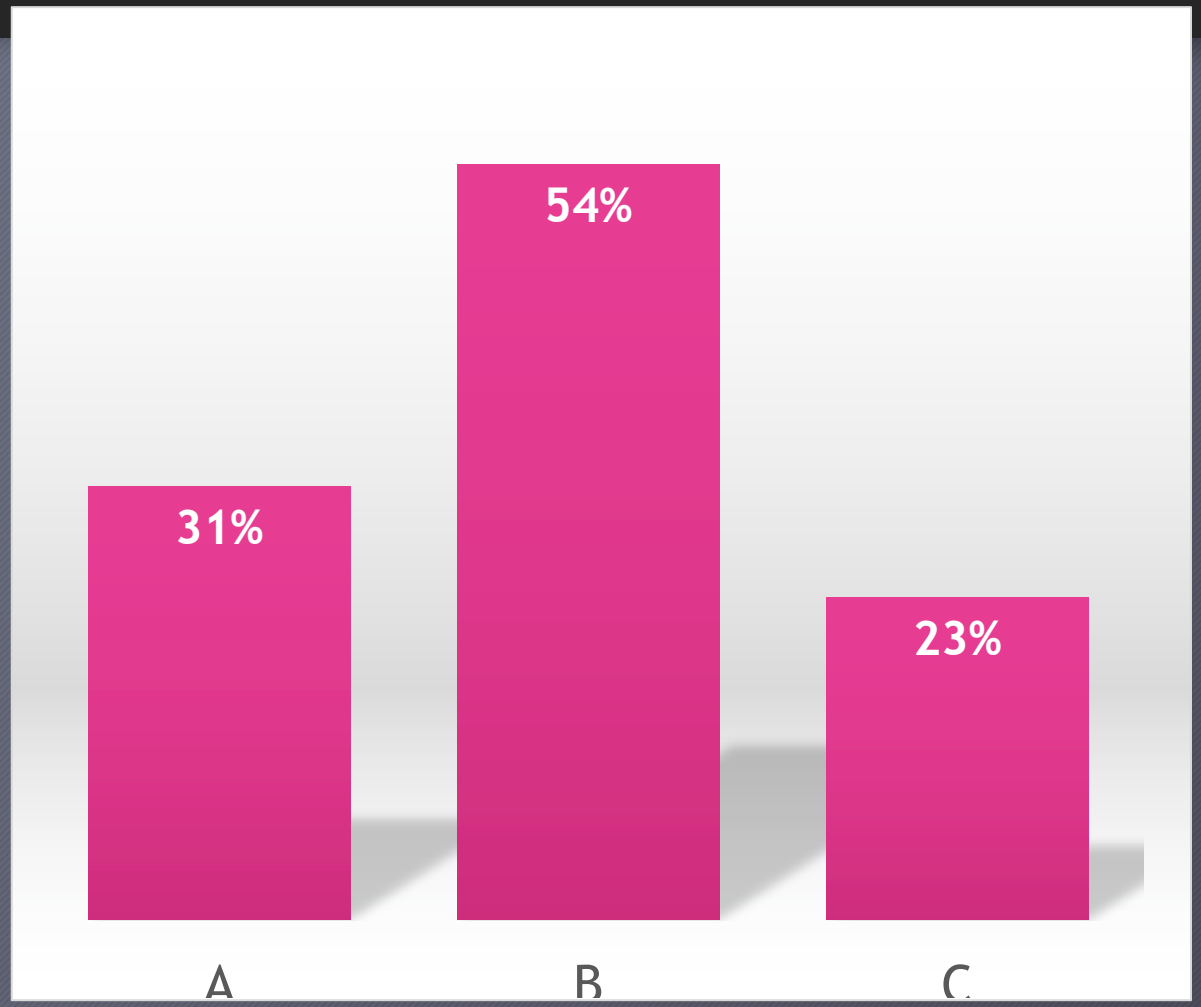
4b.
Please explain your classifications of the compounds above. A 2-3 sentence explanation will suffice.

4c.
How confident are you in your answers to 4a and 4b? 0 = not confident at all, 5 = completely confident

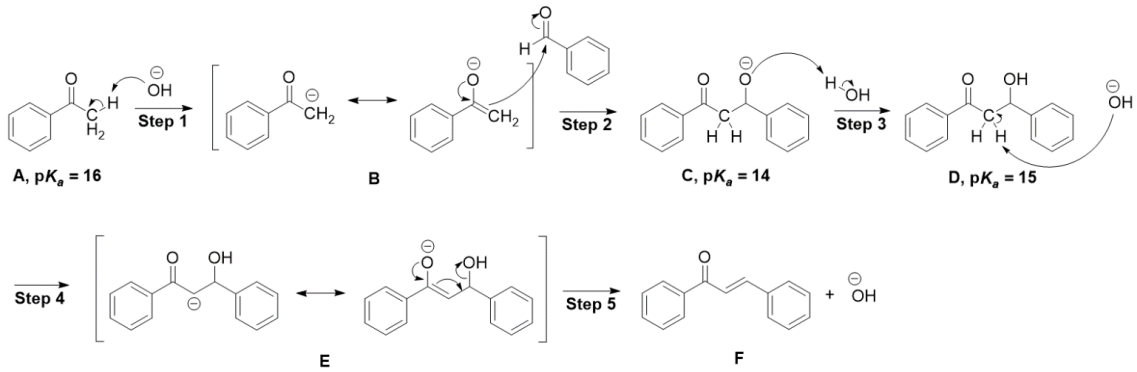
0 1 2 3 4 5

Confidence Level

Organic Chemistry I Survey



The following questions refer to the mechanism shown above. The steps of the reaction are labeled under the reaction arrows. The compounds are labeled A-F and relevant pKa values are provided. Please assume the pKa of water is 14.



5a. For Step 1, which side of the equilibrium will be favored?
Products A
Reactants B
Equally favored

5b. For Step 3, which side of the equilibrium will be favored?
Reactants C
Products D
Equally favored

5c. For Step 4, which side of the equilibrium will be favored?
Reactants D
Products E
Equally favored

5d.
Please justify your answers to parts a) - c), both in terms of the provided pKa values and the structures of the relevant compounds. A 2-3 sentence explanation will suffice.

5e.
How confident are you in your answers to 5a - 5d? 0 = not confident at all, 5 = completely confident

0 1 2 3 4 5

Confidence Level

Organic Chemistry I Survey

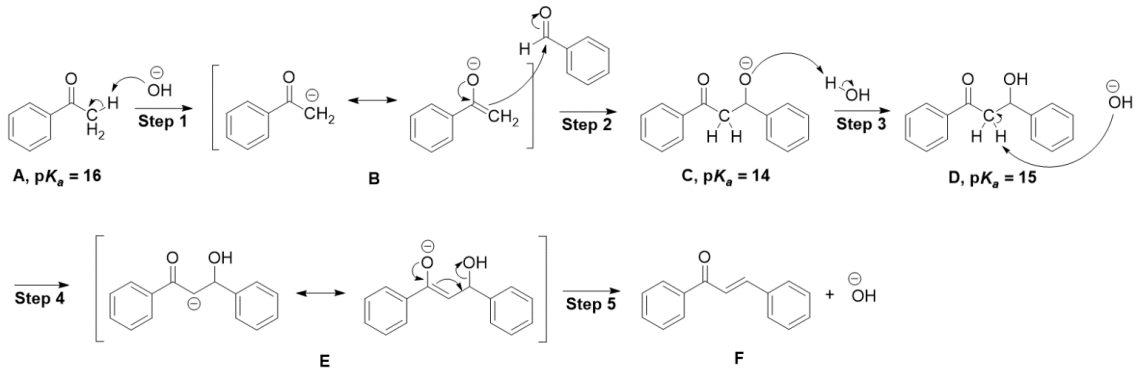
When the pKa is higher, that means that the compound is more stable. Therefore, the compounds with the highest pKa are more favored because it is more stable.

Hydroxide is a strong base, so the equilibrium will always favor the opposite side of a strong acid or base.

Stronger acids are favored

In 5a and 5c the products are favored because they have resonance stabilization. The electron density is spread through the molecule, making them weaker bases, causing that side to be favored. In 5b, products were favored because the pKa was higher, indicating weaker acids.

The following questions refer to the mechanism shown above. The steps of the reaction are labeled under the reaction arrows. The compounds are labeled A-F and relevant pKa values are provided. Please assume the pKa of water is 14.



5a. For Step 1, which side of the equilibrium will be favored?
Products A
Reactants B
Equally favored

5b. For Step 3, which side of the equilibrium will be favored?
Reactants C
Products D
Equally favored

5c. For Step 4, which side of the equilibrium will be favored?
Reactants D
Products E
Equally favored

5d.
Please justify your answers to parts a) - c), both in terms of the provided pKa values and the structures of the relevant compounds. A 2-3 sentence explanation will suffice.

5e.
How confident are you in your answers to 5a - 5d? 0 = not confident at all, 5 = completely confident

0 1 2 3 4 5

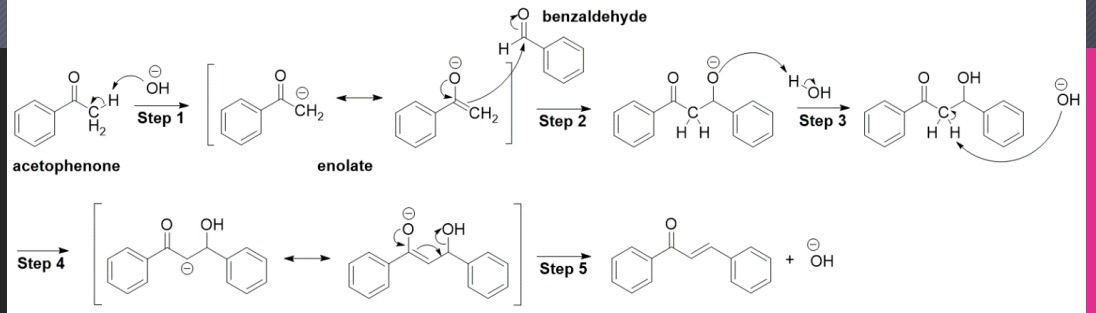
Confidence Level

Organic Chemistry II Survey

Students with almost 100% accuracy were able to Identify the role of the four species in the reaction.

However, only 20% identified the first step as being the least thermodynamically favored.

The following questions refer to the mechanism shown below. The steps of the reaction are labeled with numbers under the reaction arrows.



5a.
What is the role of hydroxide in step 1?

Brønsted Acid
Brønsted Base
Electrophile
Nucleophile

5b.
What is the role of acetophenone in step 1?

Brønsted Acid
Brønsted Base
Electrophile
Nucleophile

5c.
What is the role of the enolate in step 2?

Brønsted Acid
Brønsted Base
Electrophile
Nucleophile

5d.
What is the role of benzaldehyde in step 2?

Brønsted Acid
Brønsted Base
Electrophile
Nucleophile

5e.
Which step of this reaction is the least thermodynamically favorable?

Future Directions