

## Supporting Information: S1 Examples of Assessment Tasks

### Acid-Base Reactions – Constructed Response

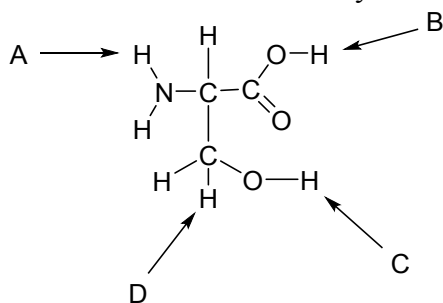
Learning Objective: Construct an explanation about why one compound is more acidic or basic than another and support your answer using your knowledge of molecular structure, electronegativity, and the stability of the conjugate acid or base.

Core idea: Structure Property relationships

Practice: Explanation

Crosscutting Concept: Cause and Effect

- a) Give at least two factors that can affect the acidity of a particular hydrogen?  
b) This compound is the essential amino acid serine. Which of the hydrogens indicated is the most acidic? Support your answer by drawing structures and by discussing the factors that affect the acidity.



- c) Which of the hydrogens is least acidic? Support your answer by drawing structures and by discussing the factors that affect the acidity.

### Acid-Base Reactions – Selected Response

Learning Objective: Construct an explanation about why one compound is more acidic or basic than another and support your answer using your knowledge of molecular structure, electronegativity, and the stability of the conjugate acid or base.

Core idea: Structure Property relationships

Practice: Explanation

Crosscutting Concept: Cause and Effect

Which is a stronger acid,  $\text{CH}_3\text{CH}_2\text{OH}$  or  $\text{CH}_3\text{CH}_2\text{NH}_2$ ? Why? (Select the correct combination of Claim, Evidence, Reasoning)

Claim:

- I.  $\text{CH}_3\text{CH}_2\text{OH}$   
II.  $\text{CH}_3\text{CH}_2\text{NH}_2$

Evidence:

- III. Oxygen is more electronegative than nitrogen  
IV. Nitrogen is a stronger base than oxygen

Reasoning:

- V. The O-H bond is more polarized
- VI. Oxygen can support the negative charge on the resulting conjugate base better
- VII. Nitrogen is better able to support the negative charge
- VIII. The N-H bond is weaker

### Acid-Base Reactions – Selected Response

Learning Objective: Discuss the factors that affect relative rates of reaction for nucleophiles and leaving groups (i.e. predict and explain trends in nucleophile strength and leaving group ability for a given set of reagents).

Core ideas: Structure Property relationships, Change and Stability

Practices: Explanation

Crosscutting Concept: Cause and Effect

Which do you predict is a better leaving group,  $\text{NH}_2$  or  $\text{NH}_3$ ? Why?

- A.  $-\text{NH}_2$  because it is a stronger base and therefore more stable
- B.  $-\text{NH}_2$  because the bond to the N is more polarized
- C.  $\text{NH}_3$  because it is a weaker base and therefore more stable
- D.  $\text{NH}_3$  because it is more polarizable

### Spectroscopy – Selected Response

Learning Objective: Explain how and why  $^1\text{H}$  NMR can be used to identify the number of non-chemically equivalent hydrogens in a compound, using their chemical shift and connectivity of adjacent carbons from the splitting pattern.

Core ideas: Structure Property relationships, Energy

Practices: Explanation

Crosscutting Concept: Cause and Effect

In the  $^1\text{H}$  NMR spectrum of acetaldehyde, the hydrogen attached to the carbonyl carbon appears:

- I at high field
- II at low field

**Because:**

- III. The electron density is low near the carbonyl carbon making the induced magnetic field in this area weaker
- IV. The electron density is high near the carbonyl carbon making the induced magnetic field in this area stronger

**And therefore**

- V. it is easier to bring the hydrogen nucleus to resonance
- VI. it is harder to bring the hydrogen nucleus to resonance

### Spectroscopy - Recitation Example

Students are re-asked a question that was on their previous examination and asked to develop grading key. They are then provided with an answer key and asked to make any necessary modifications to their grading key. Finally, we asked them to use it to grade (actual) deidentified student responses from a prior year.

Learning Objective: Explain how and why IR spectroscopy can be used to identify functional groups.

Core Ideas: Structure/Property

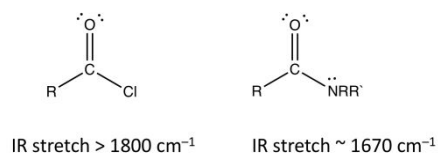
Practices: Evaluating and Communicating Information

CCC: Stability and Change

#### Instructions to student:

1. Construct a correct answer to the question
2. Use it to develop a grading key (out of 5 points) for each question. Make sure you specify which parts of your answer are necessary

Explain why the carbonyl peak of an amide appears at a different wavenumber than that of an acid chloride.



#### Answer key: (Provided Separately)

Infrared spectroscopy measures the energy that it takes to make a bond vibrate. The stronger the bond, the more energy it takes to promote that bond to a higher vibrational energy state, because more energy is needed to overcome the attractions between the two nuclei and the electrons in the bond. The amide carbonyl peak appears at a lower wavenumber than the acid chloride carbonyl peak, indicating that less energy is needed to stretch the double bond of the amide carbonyl. This is because the carbonyl double bond has more single bond character in the amide than in the acid chloride. The lone pair on the amide nitrogen interacts with the carbonyl carbon to form a species in which there is less C=O character and more C=N character than indicated by a simple Lewis structure.

#### Next Step: Student responses provided

1. Now grade each student response a score (out of 5). You should indicate why points were removed.
2. Point out incorrect statements and material in the answer that is not relevant.

#### Student responses to grade:

*“The lone pair on the N can more easily donate electrons to other atoms making it more stable where as the chlorine just stays where it is. its also easier to vibrate a single bond than a double bond, so stronger double bonds appear more downstream”*

*“There would be different peaks on the IR spectrum because there are different elements at different wavelengths when run through an IR spec. There are more bonds in the amide making it less reactive so therefore a smaller wavelength. Also the Cl on the acid chloride has more electron lone pairs and is more likely to leave as a leaving group.”*

*“A higher IR spectra indicates that a bond is harder to stretch. This means there is a stronger bond in the acid chloride than in the amide. The reason for this can be seen when we observe the amide (see picture). In the amide, the nitrogen is able to donate its electron pair to its bond with carbon, making the O negatively charged. This resonance causes the double bond between C and O to behave less like a double bond and more like a single bond. Thus, it is easier to stretch. Acid chloride, however, is a polarized molecule because the chloride is very electronegative. This makes the double bond between C and O even stronger, making it harder to stretch.”*

### **Spectroscopy – Recitation Example**

Learning Objective: Identify compounds from their IR,  $^{13}\text{C}$  NMR, and  $^1\text{H}$  NMR spectra and molecular weight and justify your answer.

Core Ideas: none

Practices: Analyzing and Interpreting data, Engaging in arguments from evidence

CCC: none

Students are provided with an IR, an  $^{13}\text{C}$  NMR, and  $^1\text{H}$  NMR and then asked the following questions.

1. What functional group(s) are present in the compound? How do you know?
2. How many different kinds of carbon are present in the molecule? How do you know?
3. Why don't all carbons appear at the same part of the  $^{13}\text{C}$  NMR spectrum (i.e. why are they spread out?)
4. How many different kinds of hydrogens appear in the  $^1\text{H}$  NMR spectrum?
5. What do the splitting patterns on the  $^1\text{H}$  NMR signals tell you about which hydrogens might be on adjacent carbons?
6. Draw a structure consistent with the spectral evidence above.
7. Label the carbons in your structure and match them to the peaks in the  $^{13}\text{C}$  NMR. Do the same with the hydrogens and the  $^1\text{H}$  NMR.

### **Spectroscopy – Recitation Example**

Learning Objective: Predict what major peaks in IR,  $^{13}\text{C}$  NMR, and  $^1\text{H}$  NMR spectra would be for simple compounds.

Core Ideas: none  
Practices: Planning investigations  
CCC: none

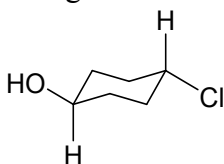
1. Draw three structures for  $C_3H_6O$
2. How would you distinguish between these three compounds using spectroscopic techniques? Describe the aspects of each technique (or spectrum) that would allow you to differentiate between the structures.

### Conformation and Configurations – Constructed Response

Learning Objective: Construct representations to explain why cycloalkanes have differing stabilities using angle strain, torsional strain and steric strain to support your argument.

Core ideas: Structure Property relationship, Change and Stability, Energy  
Practices: Modeling, Explanation  
Crosscutting Concept: Cause and Effect

- a) Draw the most stable chair conformation of *trans*-1-*t*-butyl-3-methyl cyclohexane.
- b) Draw another chair conformation that is less stable and use it to help you explain why the conformation you drew for part a is more stable than any other possible conformations.
- c) Here is a representation of *trans*-4-chlorocyclohexanol. It is chiral, label the configuration at both chiral carbons.



- d) Now draw a diastereomer of this compound and use your two representations to explain why diastereomers can be separated because they have different properties.

### Conformation and Configurations – Selected Response

Learning Objective: Construct potential energy curves for compounds showing how the energy changes as groups move closer and further apart. Explain why this happens.

Core ideas: Electrostatic Forces and Bonding Interactions, Energy  
Practices: Explanation  
Crosscutting Concept: Cause and Effect

If we look at a Newman projection of butane down the C2-3 bond, as the **dihedral angle between the two methyl groups** changes **from 60° to 0°**, what happens to the potential energy and why?

- A. The potential energy falls because there is an attraction between the electron clouds in the methyl groups
- B. The potential energy rises because there is an attraction between the electron clouds in the methyl groups
- C. The potential energy falls because there is a repulsion between the electron clouds in the methyl groups
- D. The potential energy rises because there is a repulsion between the electron clouds in the methyl groups

### Nucleophilic Substitution and Elimination – Constructed Response

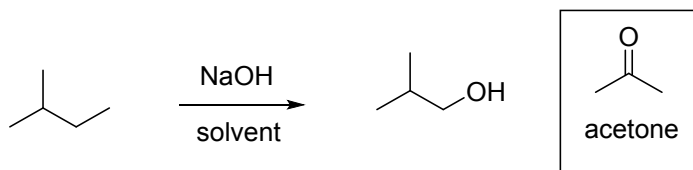
Learning Objective: Explain the role of the solvent in each of these reaction types:  $S_N2$ ,  $S_N1$ , E2, E1. Explain why a particular solvent type promotes a given reaction.

Core ideas: Structure Property relationships, Electrostatic Forces and Bonding Interactions, Energy, Change and Stability

Practices: Explanation, Modeling

Crosscutting Concept: Energy, Cause and Effect

Solvents can dramatically affect reaction rate. The  $S_N2$  reaction below proceeds approximately 2800 times faster if acetone is used as a solvent instead of methanol ( $CH_3OH$ ).



- a) Draw a molecular level diagram showing how acetone interacts (or does not interact) with NaOH. Explicitly show the role of the interactions between the solvent molecules and the relevant reactants.
- b) Draw a molecular level diagram showing how methanol interacts (or does not) interact with NaOH. Explicitly show the role of the interactions between the solvent and the relevant reactants.
- c) Succinctly explain why the reaction goes faster in acetone, being sure to reference the roles of energy and the interactions that you drew.

### Nucleophilic Substitution and Elimination – Selected Response

Learning Objectives: Explain the role of the solvent in each of these reaction types:  $S_N2$ ,  $S_N1$ , E2, E1. Explain why a particular solvent type promotes a given reaction.

Core ideas: Structure Property relationships, Electrostatic Forces and Bonding Interactions, Change and Stability

Practices: Explanation

Crosscutting Concept: Cause and Effect

$S_N2$  reactions are accelerated by which type of solvent

I.	Polar protic
II.	Polar aprotic
Because:	
III.	This solvent assists in solvating the leaving group
IV.	This solvent assists in stabilizing the carbocation
V.	This solvent solvates the nucleophile making it more reactive
VI.	This solvent does not solvate the nucleophile making it more reactive

### Nucleophilic Substitution and Elimination – Constructed Response

Learning Objective: Using molecular structure drawings, explain why the structure of the substrate determines the type of reaction. Include ideas about steric hindrance and stability of transition states and intermediates.

Core ideas: Structure Property relationships, Electrostatic Forces and Bonding Interactions, Energy, Change and Stability

Practices: Modeling, Explanation

Crosscutting Concept: Cause and Effect

- Draw a fully labeled reaction energy profile for the reaction of 2-bromobutane with  $\text{NaOCH}_3$  in DMF to produce the corresponding nucleophilic substitution product. The reaction is exergonic. Include on your profile 1) the axis, 2) the total energy change, 3) the activation energy for the rate determining step, 4) the structures of all intermediates and transition states (where necessary), and 5) the structures of the reactants and products.
- The same product would be observed if the reaction conditions were changed to warming a solution of 2-bromobutane in methanol, but the reaction energy profile would change. Draw a fully labeled energy profile for this new process.
- Explain why changing each of the conditions below causes the reaction mechanisms and reaction profiles.  
DMF  
 $\text{NaOCH}_3$   
 $\text{CH}_3\text{OH}$

### Nucleophilic Substitution – Recitation Example

Learning Objective: Describe the evidence that leads to the identification of a reaction mechanism (how do we know whether a reaction has proceeded by  $\text{S}_\text{N}1$ ,  $\text{S}_\text{N}2$ , E1, or E2). This would include thinking about kinetics, stereochemistry, and the structure of the product.

Core Ideas: Stability and Change

Practices: Using math and computation

CCC: Stability and Change

1. Imagine you have a reaction  $\text{A} + \text{B} \rightarrow \text{C}$  and you find from experiments that the rate equation is  $\text{rate} = k[\text{A}][\text{B}]$ .

- What information about the mechanism of the reaction does this equation provide?

- b) Propose a mechanism (sequence of steps or just one step) for this reaction that is consistent with the evidence.
- c) Draw a reaction energy diagram consistent with your mechanism.

### Alkenes and Alkynes – Constructed Response

Learning Objective: Predict and explain the outcome of the reversible reaction that involves addition of water to the double bond of an alkene. Discuss how you would manipulate the reaction conditions so that either the addition product or the elimination product could be obtained.

Core ideas: Structure Property relationships, Electrostatic Forces and Bonding Interactions, Energy, Change and Stability

Practices: Modeling, Explanation

Crosscutting Concept: Cause and Effect, Stability and Change

- a) Draw a fully labeled reaction energy profile for the reaction of 2-methylpropene with aqueous acid at low temperatures to produce the corresponding addition product tert-butanol. This reaction is exergonic. On your group show 1) the axis labels, 2) the overall Gibbs energy change, 3) the activation energy for the rate determining step, 4) the structures of all intermediates and transition states (where necessary), and 5) the structures of the reactants and products.
- b) The reverse reaction described above can be induced by heating the product in concentrated acid. Draw a mechanism for this reaction.

### Alcohols, Thiols and Amines – Selected Response

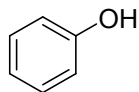
Learning Objective: Construct explanations about relative acidities of alcohols using resonance and induction arguments about the stability of the conjugate bases.

Core ideas: Structure Property relationships, Electrostatic Forces and Bonding Interactions, Energy, Change and Stability

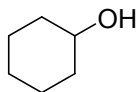
Practices: Explanation

Crosscutting Concept: Cause and Effect

Which compound is most acidic?



A. phenol



B. cyclohexanol

The reason for your answer is:

- A. Because the negative charge on the conjugate base is stabilized by induction, which makes it more stable



- B. Because the negative charge on the conjugate base is stabilized by resonance delocalizing, which makes it more stable
- C. Because the O-H bond is more polarized, so it is more reaction
- D. Because the negative charge is localized on oxygen in both compounds and therefore both are equally basic

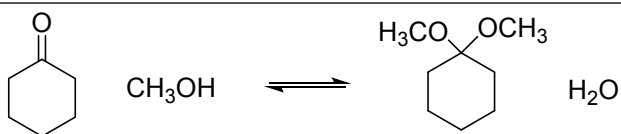
### Nucleophilic Attack at Carbonyl Carbons – Constructed Response

Learning Objective: Explain how to control a reversible reaction to produce the required materials (product or reactant).

Core ideas: Change and Stability, Structure Property relationships, Electrostatic Forces and Bonding Interactions

Practices: Explanation

Crosscutting Concept: Cause and Effect



When cyclohexanone is reacted with methanol a reversible reaction can occur to form the corresponding acetal.

- Provide two changes in condition that would increase the yield of acetal and explain why this change affects the amount of product (restating Le Chatelier's principle is not sufficient).
- If you wanted to hydrolyze the acetal back to the ketone, what conditions would you use?
- Draw a mechanism for this hydrolysis.

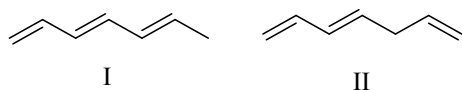
### Conjugated Compounds and Aromaticity – Selected Response

Learning Objective: Explain how and why UV-VIS spectra evidence of conjugation and identify chromophores in systems.

Core ideas: Structure Property relationships, Energy

Practices: Explanation

Which system would absorb light of the longest wavelength?



Because:

- It has the longest conjugated system
- It has the shortest conjugated system

And therefore:

- The energy gap between the HOMO and the LUMO is greatest

D. The energy gap between the HOMO and the LUMO is smallest

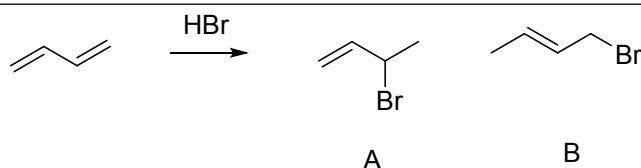
### Conjugated Compounds and Aromaticity – Constructed Response

Learning Objectives: Construct and use representations of starting materials, intermediates, transition states and products to explain how some reactions produce both kinetic and thermodynamic products. Use these explanations to predict reaction conditions that would favor kinetic or thermodynamic control of the reaction.

Core ideas: Structure Property relationships, Electrostatic Forces and Bonding Interactions, Energy, Change and Stability

Practices: Modeling, Explanation

Crosscutting Concept: Cause and Effect



- Construct a mechanism using curved arrows for the formation of products A and B
- Draw an energy diagram for the formation of both products A and B. Explicitly label the reactants, products, activation energies, and the structure(s) of any intermediates.
- Which product would predominate at low temperatures? Explain your choice using your mechanism from Part a, your graph in Part b and drawing on your knowledge of energy, molecular structure, and electrostatic forces.

### Conjugated Compounds and Aromaticity – Selected Response

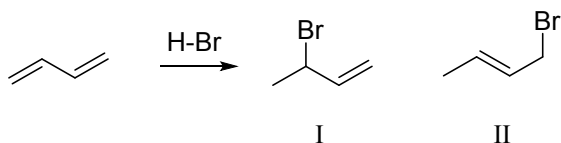
Learning Objectives: Construct and use representations of starting materials, intermediates, transition states and products to explain how some reactions produce both kinetic and thermodynamic products. Use these explanations to predict reaction conditions that would favor kinetic or thermodynamic control of the reaction.

Core ideas: Structure Property relationships, Electrostatic Forces and Bonding Interactions, Energy, Change and Stability

Practices: Explanation

Crosscutting Concept: Cause and Effect

Which product is formed at the lowest temperature?



Because:

III. the intermediate formed from addition of the electrophile ( $\text{H}^+$ ) is more stable

IV. The transition state as the  $\text{Br}^-$  adds is of lower energy

### Returning to the Carbonyl – Constructed Response

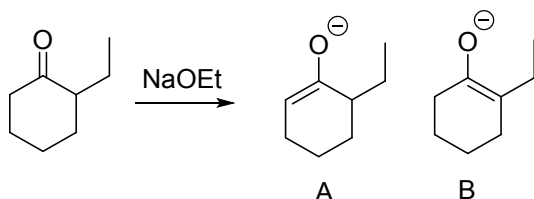
Learning Objective: Construct energy diagrams to show how kinetic or thermodynamic products can be formed by alkylation at the alpha carbon.

Core ideas: Structure Property relationships, Electrostatic Forces and Bonding Interactions, Energy, Change and Stability

Practices: Modeling

Crosscutting Concept: Cause and Effect

Two enolates can be formed from the treatment of 2-ethylcyclohexan-1-one by  $\text{NaOEt}$



- Draw a fully labeled reaction energy profile depicting the formation of both enolates from 2-ethylcyclohexan-1-one (show enolate A as a dotted line and enolate B as a solid line). On your graph include 1) axis labels, 2) the activation energy for the rate determining step for each enolate, 3) where the two enolates A and B are on the diagram, and 4) the difference in energy between the two enolates.
- Treatment of 2-ethylcyclohexan-1-one with  $\text{NaOEt}$  followed by heating the reaction mixture will mostly produce one of the enolates listed in Part a. Which will be formed? A or B?
- Explain why this enolate is formed more slowly (why heating is necessary) using forces and energy in your explanation and why it is more stable.