MOQ 2 solutions

Question a(i) Blank 1 was not graded and your MOQ 2 grade was based on a total of 4.5 instead of 5. Divide your MOQ 2 total by 4.5 instead of 5 to determine your %. 80% or higher = pass (master).

The structures of reactants, intermediates, and products gives us information about energy, stability, and reaction rate, and helps us predict the product of a reaction or explain the product distribution.

a. Carotene is the orange pigment in carrots. It absorbs visible and UV light and works as an antioxidant to protect plant cells from the destructive effects of UV radiation. You eat your carrots but what happens when carotene reacts with stomach acid?

Compound A is part of the conjugated pi system of carotene. Compound A reacts with HCl to form Compound B and Compound C.

Set 1 shows the resonance structures when HCl reacts with the C=C pi bond in the ring.

Set 2 shows the resonance structures when HCl reacts with the right C=C pi bond in the chain.

Set 3 shows the resonance structures when HCl reacts with the left C=C pi bond in the chain.

(i) The Set 1 resonance structures will NOT likely form because___.

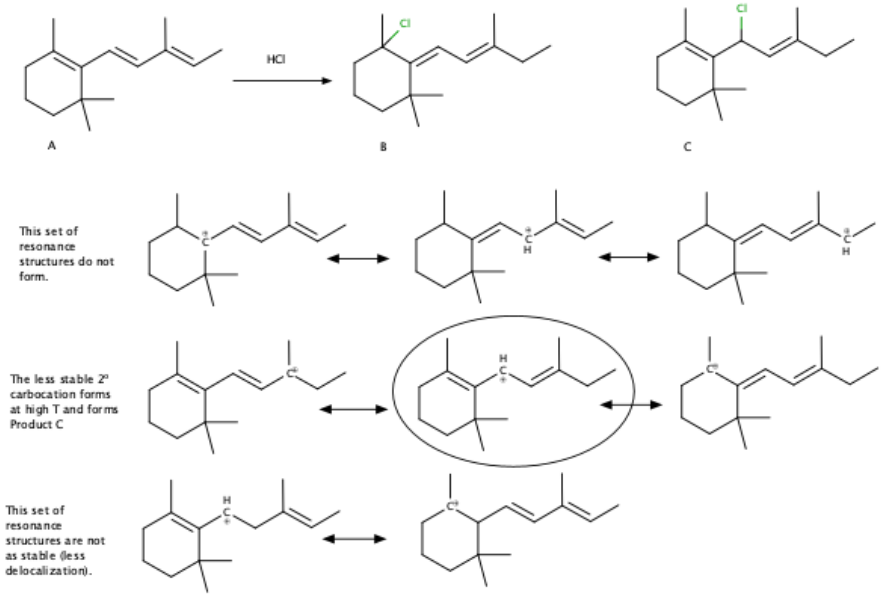
MISTAKE: 3º allylic carbocation shown is more stable than the 3º carbocation that could also form. This question was not graded and your MOQ 2 grade was based on a total of 4.5 instead of 5.

The Set 2 resonance structures are ___ stable than the Set 3 resonance structures. (Answer: more or less or same.)

(ii) This reaction occurs at 37ºC (body temperature) so the major product is C. (Answer: B or C)

Circle the resonance structure that produces the major product and explain why this intermediate forms at body temperature.

37ºC (body temperature) is considered high temperature (vs. 0ºC low temperature) so more of the higher energy, less stable 2º carbocation intermediate forms, which makes Product C.



b. You synthesize Compound Y from benzene.

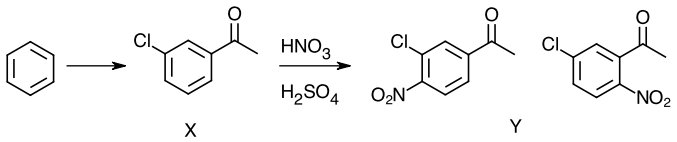
(i) To make Compound X, I would ___ because ___.

substitute Cl first, followed by $COCH_3$ (blank 1)

substitute $COCH_3$ first, followed by Cl (blank 1)

Blank 2: give reasons. $COCH_3$ is a meta director whereas Cl is an o, p director.

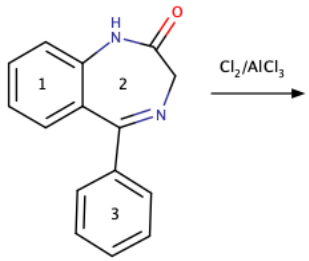
(ii) Draw the structure of Compound Y. Explain why this product forms from Compound X.



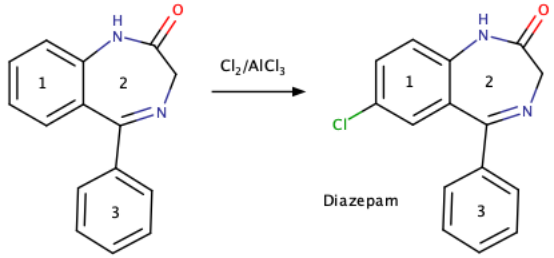
X Y

Cl is the stronger activating group and is an ortho, para director. $COCH_3$ is the weaker activating group and is a meta director.

c. You are synthesizing a possible drug at your new job at the pharmaceutical company.

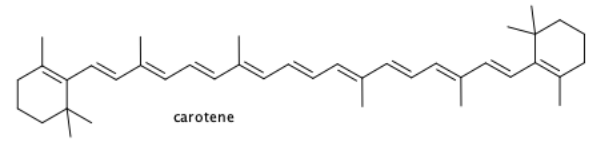


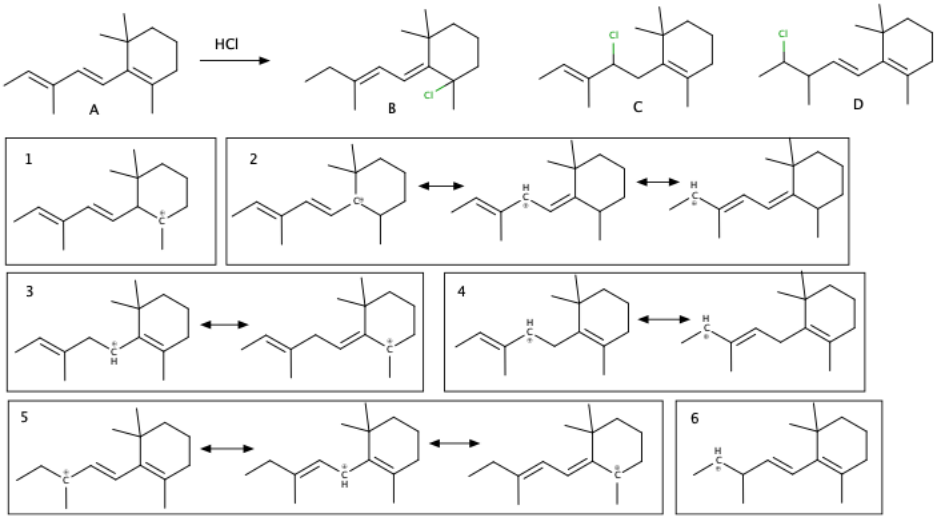
(i) Electrophilic aromatic substitution (EAS) reaction occurs at Ring(s) 1 and 3.
(ii) EAS occurs at Ring 1 because ___. If your answer to Blank 1 involves more than one ring, compare the two rings and explain why EAS occurs at one ring and not the other.
the N (amide group) and C (imine group) atom(s)/group(s) activates this ring better than the C (imine group) atom(s)/group(s) in Ring 3 and forms reacts faster
Draw the structure of the product.



Diazepam (Valium) is a prescription drug to treat anxiety.

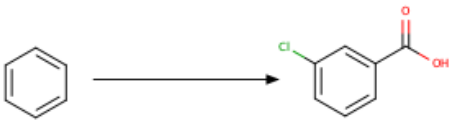
Multi-Objective Question 2 retake solutions
The structures of reactants, intermediates, and products gives us information about energy, stability, and reaction rate, and helps us predict the product of a reaction or explain the product distribution.
a. Carotene is the orange pigment in carrots. It absorbs visible and UV light and works as an antioxidant to protect plant cells from the destructive effects of UV radiation. You eat your carrots but what happens when carotene reacts with stomach acid?
Compound A is part of the conjugated pi system of carotene. Compound A reacts with HCl to form Compound B, Compound C, and Compound D.
Six possible intermediates are shown below.





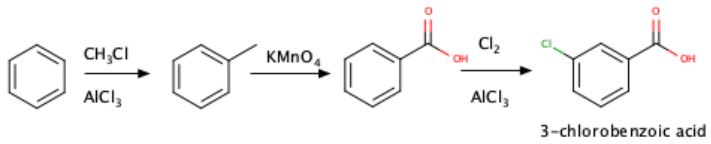
(i) The most stable intermediate is/are 2 and 5 because 3º allylic carbocations. The least stable intermediate is/are 6.
Blanks 1 and 3: give a number(s) only.
1, 2, 3, and 5 are 3º allylic carbocations.
2 and 5 are the most stable 3º allylic carbocations because the + charge and pi electrons are delocalized over the most atoms (5 in each case as shown by 3 resonance structures).
1 and 3 are less stable 3º allylic carbocations because the + charge and pi electrons are delocalized over the fewer atoms (3 in each case as shown by 2 resonance structures).
(ii) This reaction occurs at 37ºC (body temperature) so the major product is D. Intermediate 6 forms at body temperature because more of the higher energy intermediate forms at body temperature than at 0ºC.
Blank 1: answer B or C or D. Blank 2: give a number only. Blank 3: give a one word answer.

b. You are studying the properties of Wellbutrin (antidepressant and smoking cessation drug) and find 3-chlorobenzoic acid (m-chlorobenzoic acid) is a metabolic byproduct of this drug. You want to synthesize 3-chlorobenzoic acid from benzene.

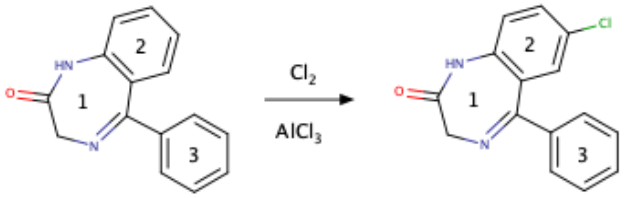


3-chlorobenzoic acid

(i) To make 3-chlorobenzoic acid, I would ___ because ___ is a meta director.
substitute Cl first, followed by COOH (blank 1)
substitute COOH first, followed by Cl (blank 1)
substitute CH_3 first, oxidize CH_3 to COOH, followed by Cl (blank 1)
substitute CH_3 first, followed by Cl, and oxidize CH_3 to COOH, (blank 1)
substitute Cl first, followed by CH_3, and oxidize CH_3 to COOH (blank 1)
Blank 2: give an atom or group.
COOH
(ii) Show the reaction conditions and product for each step of your synthesis of 3-chlorobenzoic acid from benzene.



c. You are synthesizing a possible drug at your new job at the pharmaceutical company.



(i) Electrophilic aromatic substitution (EAS) reaction will not occur at Ring(s) 1. Give a number only.
(ii) Ring 3 is bonded to a carbon in Ring 1. Ring 3 is less activated than Ring 2. This tells me EAS occurs at Ring 2.
Blank 1: answer more or less or same. Blank 2: give a number only. Blank 3: give a number only.
Draw the structure of the product.
The product is Diazepam (Valium) - a prescription drug to treat anxiety.

Quiz 6 solutions

1. Benzene reacts with an electrophile, E^+. Compared to a simple pi bond, the pi bonds in benzene are ___ nucleophiles because benzene is ____. E^+ has to be a ____ electrophile. Give a one word answer in each blank.

Weaker, aromatic, Strong

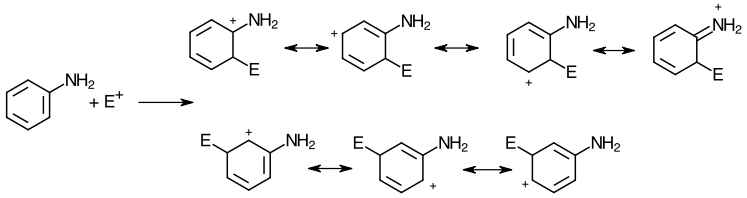
2. Aniline ($C_6H_5NH_2$) reacts with E^+ in an electrophilic aromatic substitution (EAS) reaction. The intermediates that form in the ortho and meta positions are shown.

a. Draw the other resonance structures for the ortho intermediate. Which structure is the most stable?

3 additional resonance structures. Most stable resonance structure is the 2° carbocation bonded to N. The other 2° carbocations are bonded to H, which are less stable. The N distributes the + charge better than H.

b. Draw the other resonance structures for the meta intermediate. Which structure is the least stable?

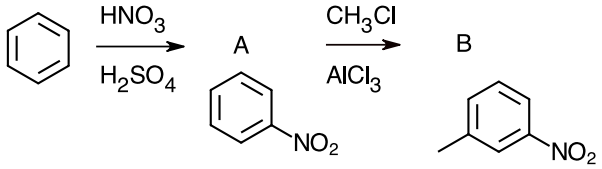
2 additional resonance structures. All are 2° carbocations and have the same stability.



c. Explain why the -NH_2 directs EAS in the ortho position and not the meta position.

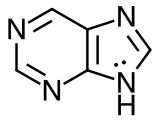
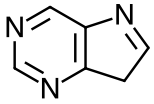
Ortho intermediate (4 resonance structures) is more stable (lower energy) and forms faster than the meta intermediate (3 resonance structures) so ortho reaction product forms faster.

3. You want to make a TNT-type compound. Draw the structures of Product A and Product B.



Quiz 5 solutions

1. a. Purine is one of the six bases found in DNA and is aromatic. Explain why purine is aromatic using the 4 aromaticity criteria. State the number of conjugated pi electrons. If any atom(s) in a ring do not have any pi bonds, state the shape (molecular geometry) of this atom.

ring

conjugated including lone pair on N bonded to H

planar ring - all atoms in rings are on the same plane. N bonded to H has a trigonal planar shape (sp^2 hybridized) with the lone pair in a p orbital.

10 electrons (8 from pi bonds + 2 from 1 lone pair) in conjugated system so fits 4n + 2 rule.

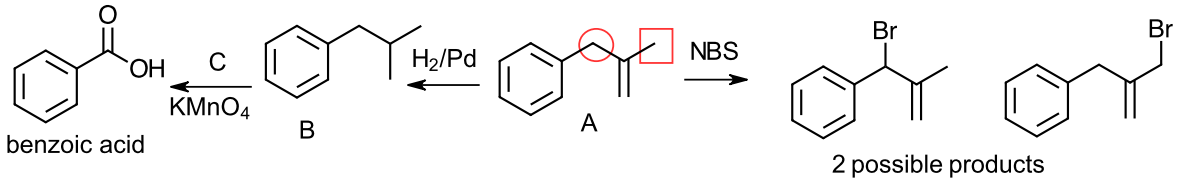
b. If one of the nitrogen atoms in purine is changed to a carbon, the resulting compound is no longer aromatic. Draw the structure of this compound. Identify the aromaticity criteria that no longer hold for this compound.

See structure above. Change N bonded to H to a C.

4n + 2 rule - Loss of lone pair reduces pi electrons to 8 and does not fit the 4n + 2 rule.

Planar ring - C is tetrahedral and makes the ring non-planar.

2. a. Circle the benzylic carbon and box the allylic carbon in Compound A. Compound A reacts with NBS to form two possible products. Draw the structures of these two products.



b. In Compound A, the C=C pi bond in the chain is ___ reactive than the C=C pi bonds in the ring because ____. This means when Compound A reacts with H_2/Pd to form Compound B, the product is ___.

Blank 1: answer more, less, or equally. Blank 2: give reasons. Blank 3: draw the structure.

The pi electrons in the aromatic ring are delocalized and more stable and less reactive than the pi electrons in the simple alkene.

c. Compound B reacts with Reagent C to form benzoic acid. Give the chemical formula of Reagent C. Identify the reaction type (acid-base, substitution, etc.)

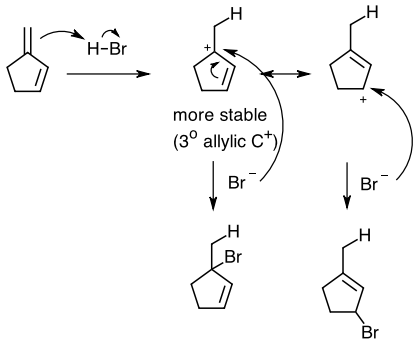
C = $KMnO_4$. Oxidation reaction.

Quiz 4 solutions

1. The 6 carbon ring compound reacts with HBr.

a. The pi bond in this compound is less reactive than the pi bond in C_2H_4 due to delocalization.

b. Use curved arrows to show how the pi bond outside the ring reacts with HBr to form an allylic carbocation intermediate.



c. Draw resonance structures of the carbocation intermediate from part b. Which resonance structure is more stable? Give reasons.
d. Draw the structures of the addition product that forms from each intermediate. Use curved arrows to show how each product forms.
e. The product that forms at 0°C is 3-bromo-3-methyl-1-cyclohexene (1,2 product) because the lower energy intermediate is formed faster than the less stable intermediate.