Midterm 1 – Chem 3A, Fall 2020
Monday, 9/28/2020, 7-9 pm

Time limit: (90 minutes for exam content) + (30 minutes for technology)
= **120 minutes** from when the file is accessed on the Gradescope site
(Note that the Gradescope site will NOT allow any file uploads after the 120 min timer has expired.)

Academic Integrity:
I acknowledge the following academic integrity guidelines for this exam:

- If I submitted an "Exam Notes" assignment on bCourses for this exam, I **AM** allowed to use those notes for this exam.
- I **AM** allowed to use a physical model kit and/or the following virtual model kit (website) during the exam: https://chemagic.org/molecules/amini.html
- I am **NOT** allowed to use any other notes or resources during the exam (including materials posted on the course website or ANY other websites.)
- I am **NOT** allowed to communicate about the questions or content of the exam with anyone other than Chem 3A instructors, directly or indirectly, until **3:00 pm PDT on Tuesday, 9/29/2020.**
  - **Zoom** link to communicate with instructors during the exam: https://berkeley.zoom.us/j/97149509861?pwd=SkppZkxiWkFmLzZDMlVEbGtpWDQ5UT09
- I am **NOT** allowed to post files or images of any part of this exam on ANY website, even after the deadline above has passed, with the exception of the Fall 2020 Chem 3A Piazza site.

Name_____ Student ID #_____

Signature: _____

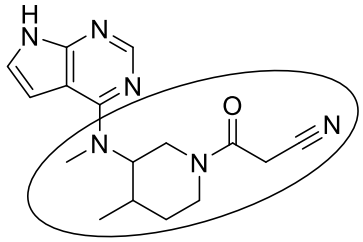
Guidelines for Using R Group Notation and Copying Structures:

Some questions require structure drawings as answers, in which parts of the structure are the same as an original given in the exam and other parts are changed. For these questions, the **entire structure**, **including parts that are unchanged from the original given in the question**, must be redrawn (correctly) in the answer to earn full credit on that answer.

- **R Group Notation** (circled/labeled groups)
  - When a question specifies that **R group notation should be used**, using the notation correctly is **required to earn credit.** Answers that do NOT use this notation correctly as specified in the question (including answers that ignore the R abbreviation and include the whole structure instead) will be marked incorrect.
  - When a question **does NOT specify that R group notation should be used**, then that type of notation is **not permitted** in the answer. The whole molecule must be drawn correctly to earn credit.
- Answers in which the "unchanged" part of a structure has a drawing error in it will be marked as incorrect.
- Copy/pasting screenshots (in digital ink versions) for the unchanged parts of structures is **not permitted**, in the interest of keeping the testing experience as similar as possible between students who are using digital ink and students who are printing and scanning the exam. Any copy/pasted structures will be marked as incorrect (as a drawing error).

The questions throughout this exam will explore the structure and several reactions in the multistep synthesis of Compound X, which is a medication.

1. **Bond Line Notation.** Count the **carbons and hydrogens** in the circled part of the structure. (2 x 2 = 4 pt)

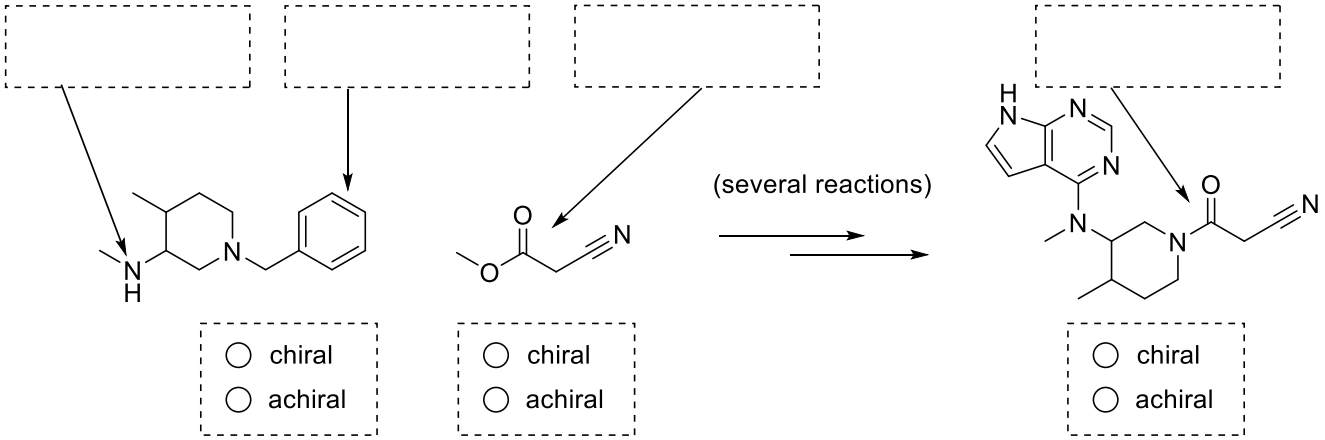


Compound X

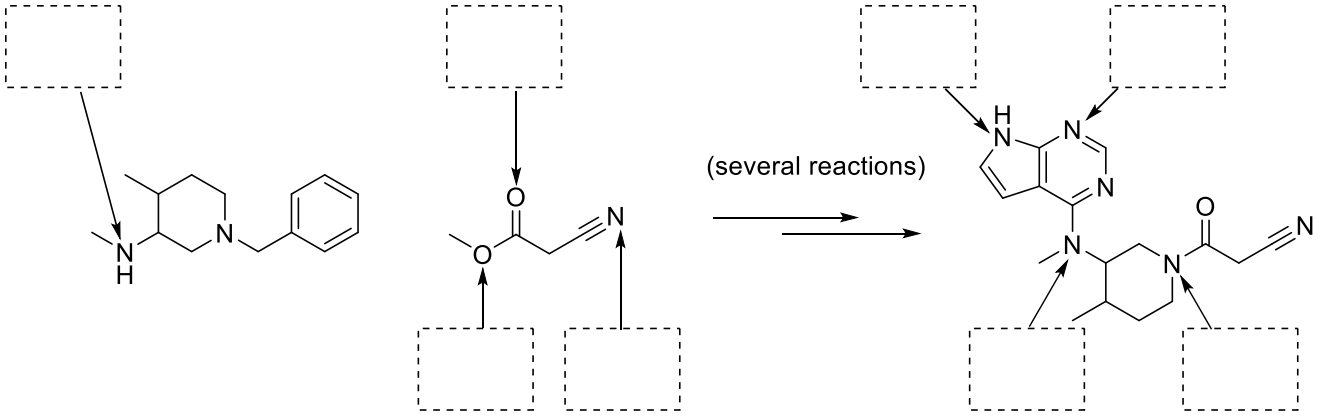
How many carbons are in the part of the structure that is circled? ☐

How many hydrogens are in the part of the structure that is circled? ☐

2. **Multistep Synthesis Starting Materials** Two of the starting materials that are used in the multistep synthesis of Compound X are shown below.
   a. Name the indicated **functional groups** in this scheme. (4 x 2 = 8 pt)
   b. Classify each structure as **chiral or achiral**. (3 x 2 = 6 pt)



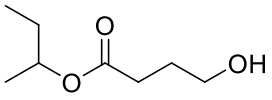
3. **Hybridization.** State the hybridization of each atom in the scheme. (8 pt)



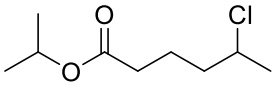
4. **Nomenclature**

a. The names of the structures below contain a functional group suffix (-oate) that was not discussed in class. Analyze the relationship between the structure and the name in the first two examples. Based on this analysis, **name the third structure** *(hint: it ends in "oate".)* (8 pt)

b. Modify each of the first two structures (turn one bond into a **wedged or dashed line**) to show the **stereochemistry** given in the name. (2 x 2 = 4 pt)

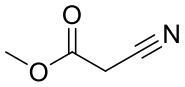


(S)-sec-butyl 4-hydroxybutanoate



(R)-isopropyl 5-chlorohexanoate

(modify to show stereochemistry using a wedged or dashed bond)



5. **Stereochemistry of Compound X**

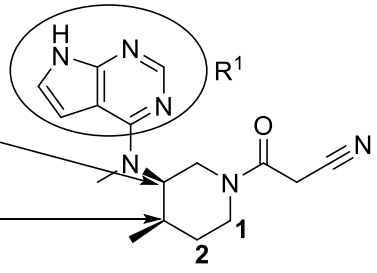
a. Indicate the **configuration (R or S)** of each stereocenter in Compound X. (2 x 3 = 6 pt)

b. As shown on the chair templates below, the carbonyl substituent on nitrogen is **neither axial nor equatorial**. Explain what causes this. (2 pt)

c. **Add substituents** to finish the two chair conformation drawings. (8 pt)

○ R ○ S

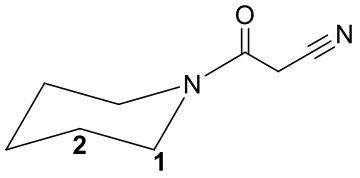
○ R ○ S

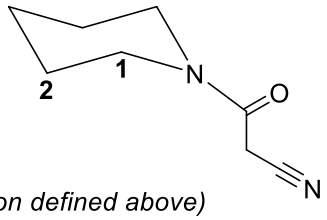


(Compound X)

The reason that the carbonyl substituent is located in a position that is neither axial nor equatorial is:

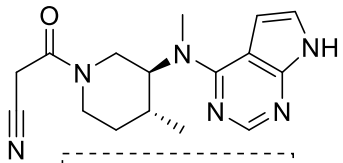
(15 words or fewer)



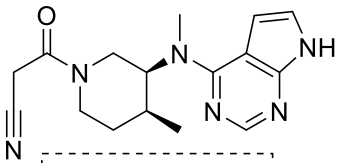


(add substituents, using the numbering and R^1 abbreviation defined above)

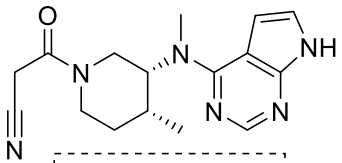
d. Indicate the **relationship** between each structure below and **Compound X (above)**. (3 x 3 = 9 pt)



○ enantiomer ○ diastereomer ○ identical



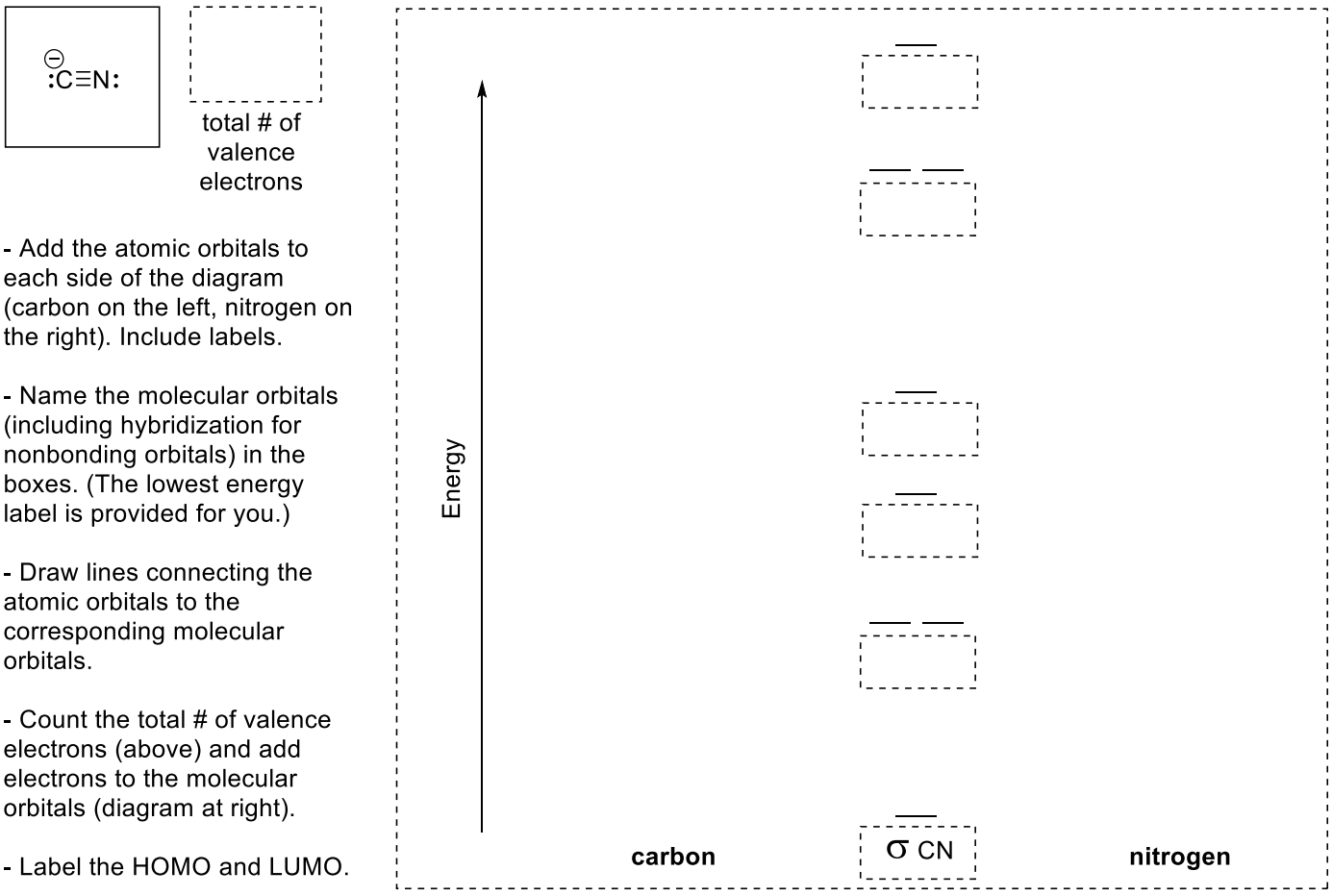
○ enantiomer ○ diastereomer ○ identical



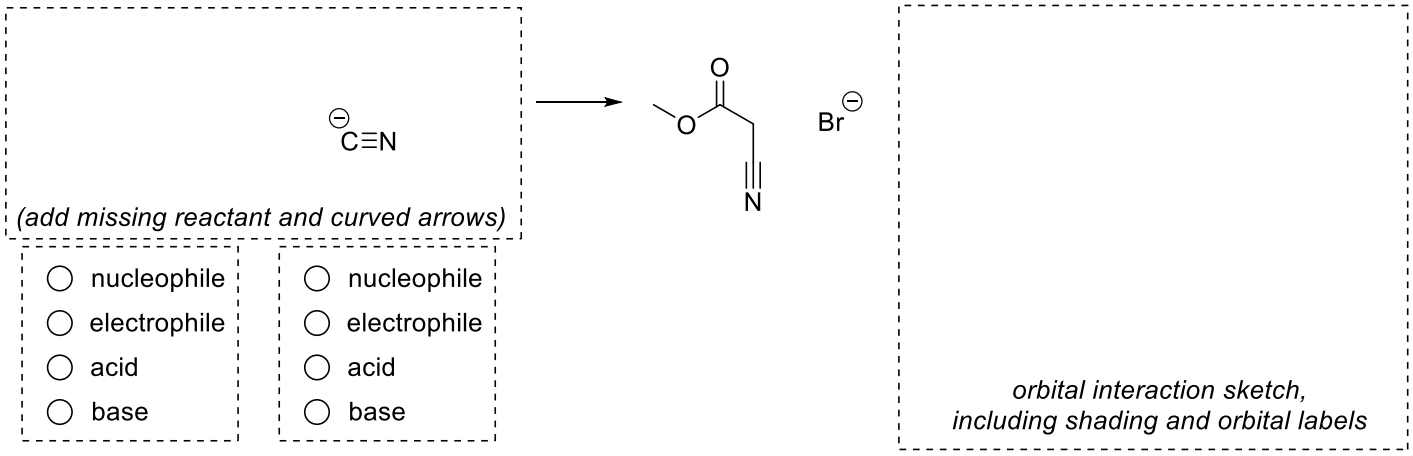
○ enantiomer ○ diastereomer ○ identical

6. **Orbital Interaction Diagram**

Count the valence electrons and finish the **orbital interaction diagram** for the ion shown in the box following the instructions in the figure. Note that this diagram **includes nonbonding electrons**. (9 pt)

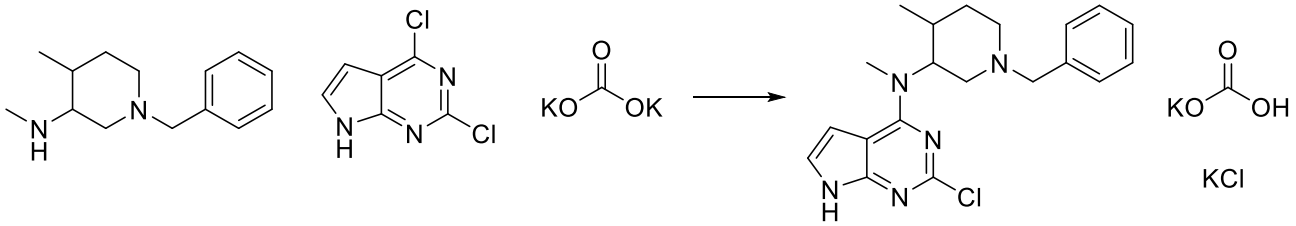


7. **Reaction A.** One of the starting materials for the synthesis of Compound X can be made using the following concerted substitution reaction.
   a. Add the **missing reactant** and **curved arrows**. (2 pt)
   b. Classify the **roles of the reactants.** (1 pt)
   c. Draw a **picture of the orbital interaction** that leads to the new bond. Include orbital shading and labels for the reactive orbitals. (2 pt)
   Note: ONLY include the reactive orbitals in the picture and use bond-line notation for the rest of each reactant molecule. (DO NOT include orbitals in the picture that are not the reactive orbitals in this mechanism.)



8. **Reaction B**. One of the reactions in the multistep synthesis of Compound X is shown below.

a. The **balanced equation for the reaction** is shown below. Compare the balanced equation in this scheme to the mechanism (part c of this question). **Circle and label the R group** on the balanced equation starting material to correspond to the abbreviated structures in the mechanism. (1 pt)



Circle and label the R group in the starting material based on the abbreviated structures in the mechanism below.

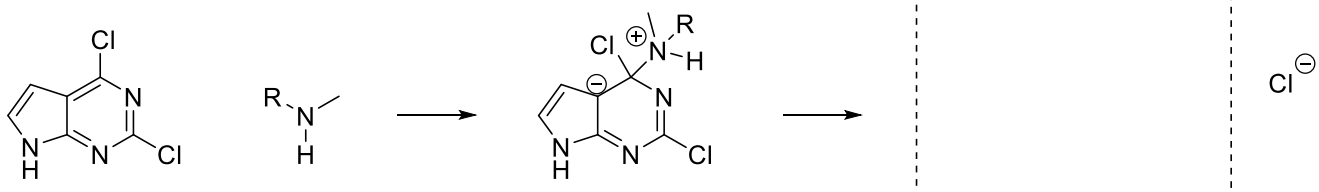
b. At least one structure in the reaction scheme above includes ionic bonding. **Redraw any/all ionic reactant(s)/product(s)** to explicitly show all lone pairs and formal charges. (5 pt)
Note: Do NOT include drawings of structures that contain only covalent bonds.

ionic reactant(s) (if any)
show all lone pairs and formal charges

ionic product(s) (if any)
show all lone pairs and formal charges

c. The **mechanism of the reaction** is shown below. Add **curved arrows** and **the missing structures** to complete the mechanism. Use the balanced equation above to help with identifying missing structures. Classify **reactant roles** for the first mechanism step. (6 pt)

Mechanism:

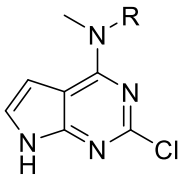


○ nucleophile	○ nucleophile
○ electrophile	○ electrophile
○ acid	○ acid
○ base	○ base

(intermediate with one formal charge)

Cl

(base)



Cl

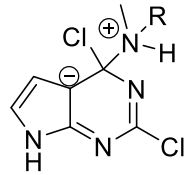
(add curved arrows throughout the whole mechanism)

9. **Resonance in Reaction B**

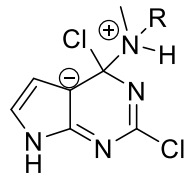
The first intermediate in the mechanism on the previous page is resonance contributor A in the scheme below. (9 pt)

a. Draw **curved arrows and resonance contributors** B, C, and D, paying careful attention to the instructions in each box.

b. Complete the statements at the right about the **ranking of the resonance contributors**.

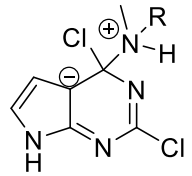


contributor A ⟷ contributor B



contributor A ⟷ contributor C

(add curved arrows) *two "major" contributors (either order)*



contributor A ⟷ contributor D

(add curved arrows) *a significant "minor" contributor*

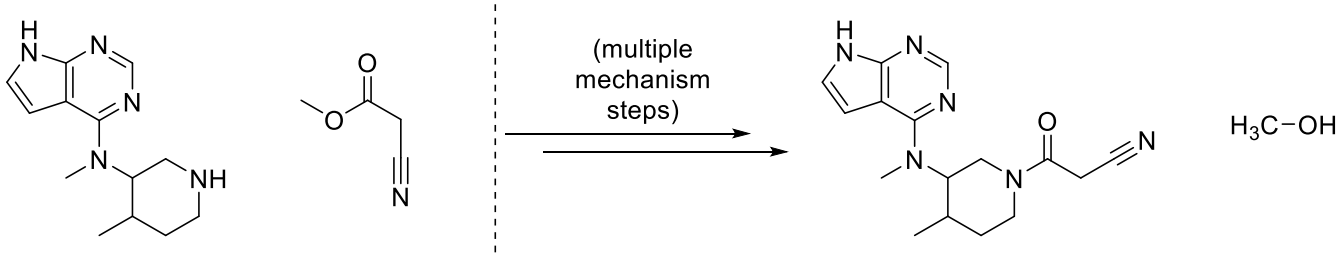
Resonance contributor A is a(n)

- ◯ major contributor
- ◯ minor contributor
- ◯ insignificant contributor

The distinction between "major" vs. "minor" contributors in this set is based on:

(10 words or fewer)

10. **Reaction C.** A later reaction in the multistep synthesis of Compound X is shown below. The scheme does not show the mechanism, but thinking about how the mechanism could possibly work, classify the **reactant roles** and circle/label the **leaving group "LG"**. (2 pt)



circle and label the leaving group "LG"

◯ nucleophile	◯ nucleophile
◯ electrophile	◯ electrophile