CHM 2120A
Midterm #1
October 13, 2021

First Name: _____ Last Name: _____

Student Number: _____

Approximate total number of marks: 65
The marks are given as a guide and are subject to minor changes.

Instructions:

1. You can write the midterm digitally, on blank paper, or on a printed copy of the midterm.
2. When finished, submit your midterm to this assignment space in PDF format. If you are scanning papers, please use a scanner or app that scans to PDF. The Dropbox app is one option.

Academic integrity rules for Midterm 1:

1. Work individually, without consulting or working with anyone else
2. Open book: you may consult text or internet sources, except where answers are explicitly posted (e.g., Discord, Chegg)
3. You may not post questions/answers or ask for answers

Important! **If you become aware of academic dishonesty** during the midterm, report it to Dr. Flynn by email or anonymously.

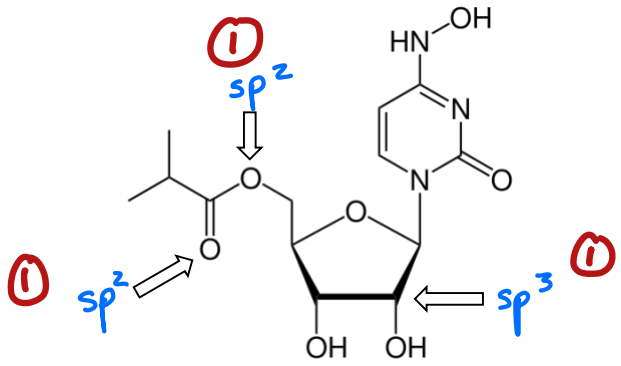
Please sign below to attest that you have read and agree to the rules for academic integrity for this midterm:

Signature: _____

- Have questions during the midterm? You can:
  - Post your question Slack (preferred)
  - Contact Dr. Flynn via Zoom (class link)
  - Email Dr. Flynn (confidential messages only)

11:24

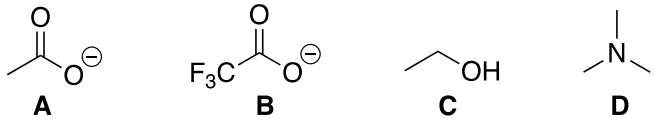
1. What is the hybridization of each of the indicated atoms in molnupiravir, Merck's new COVID drug? (3 points)



2. Rank the following compounds in order of increasing leaving group ability (worst to best) (3 points)

D < A < B < C

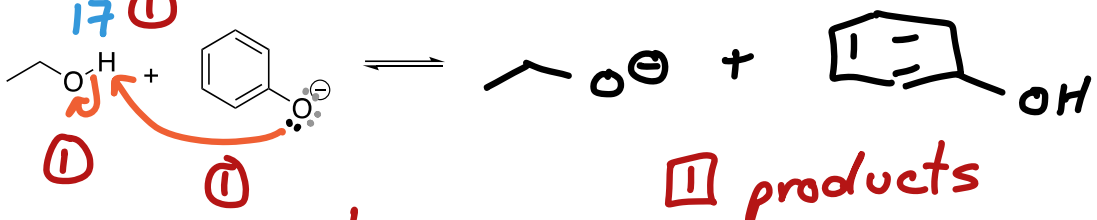
-1 per switch



3.

a. Draw the mechanism and products for the reaction below. (3 points)
b. Provide the approximate pK_a values of each acid. (2 points)
c. Predict the direction of the equilibrium. (1 point)

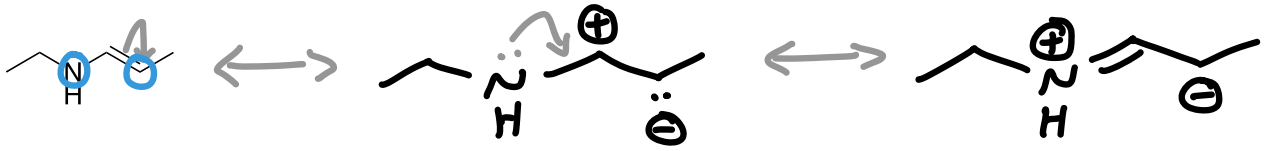
10 (±1)



(words or arrows)

4.

a. Draw two additional resonance structures for the molecule below. (2 points)



(parts in grey are not required)

1 1

b. What aspect of the resonance hybrid structure is more accurate than drawing resonance structures? (1 point)

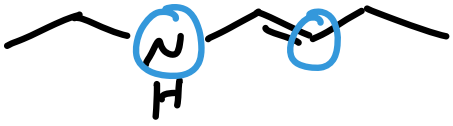
comparison needed

1 shows a mix/average/blend of resonance structures, rather than (incorrectly) alternating ones. 1

c. Circle the nucleophilic sites on the original structure. (2 points)

1 point each

switching



5.

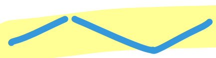
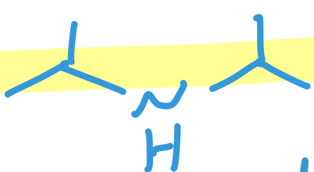
a. Compare the following bases and circle how each factor affects each base's relative stability. (5 points)

A **B**

Electronegativity	Stabilizes **A** more than **B** [circled]	Stabilizes **B** more than **A**	Not relevant
Atom size	Stabilizes **A** more than **B**	Stabilizes **B** more than **A** [circled]	Not relevant
Resonance	Stabilizes **A** more than **B**	Stabilizes **B** more than **A**	Not relevant [circled]
Hybridization	Stabilizes **A** more than **B**	Stabilizes **B** more than **A**	Not relevant [circled]
Inductive effects	Stabilizes **A** more than **B**	Stabilizes **B** more than **A**	Not relevant [circled]

b. Which factor(s) dominate the relative stability in this case? (1 point) electronegativity

c. Justify your response in **b** using multicomponent causal reasoning, using experimental evidence to support your argument. (4 points)

Based on the pKa values of the conjugate acids (experimental data),  OH is a stronger acid than  (pKa ~17 vs 38).

comparison ① than — values stated ①

 O⊖ is therefore the weaker base, indicating that electronegativity must be the dominant factor over atom size. (the multicomponent part)

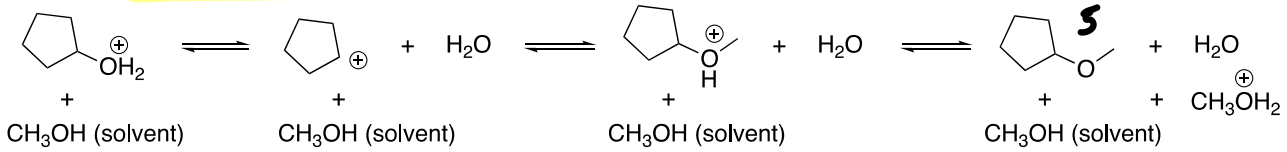
causal link ① — ①

(hence the "rule" that electronegativity factors dominate across a row in the periodic table)

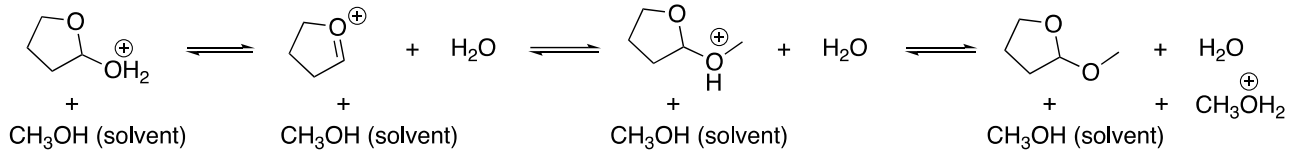
6.

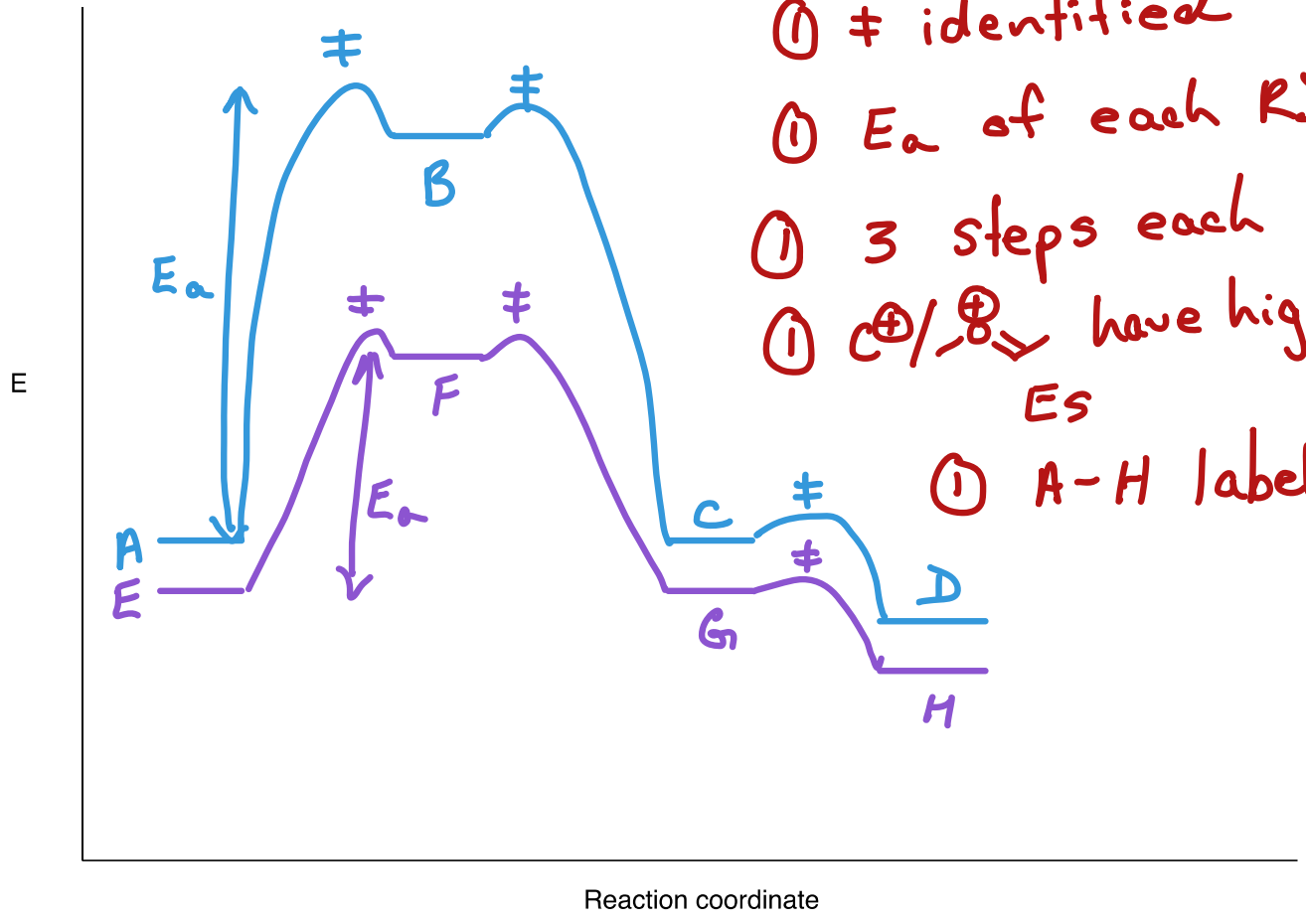
a. Draw and label the reaction coordinate diagram for reaction mechanisms **1** and **2**, including for each mechanism the: transition states, activation energy of the rate determining step, reactants, intermediates, and products, as applicable. (5 points)

(1)



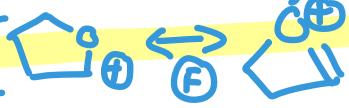
(2)





b. Which reaction would likely proceed fastest? _____ (1 point)

c. Justify your answer in part b, using your reaction coordinate diagram as part of your explanation and at least linear causal reasoning. (3 points)

The ① E_a of the RDS is lower for reaction 2 than 1. ① The t.s. of the RDS is lower E, being approximated by the carbocation's structure (Hammond postulate). The resonance stabilized carbocation  is more stable/lower E than ① the 2° C⊕ (B). The rxn with to lowe

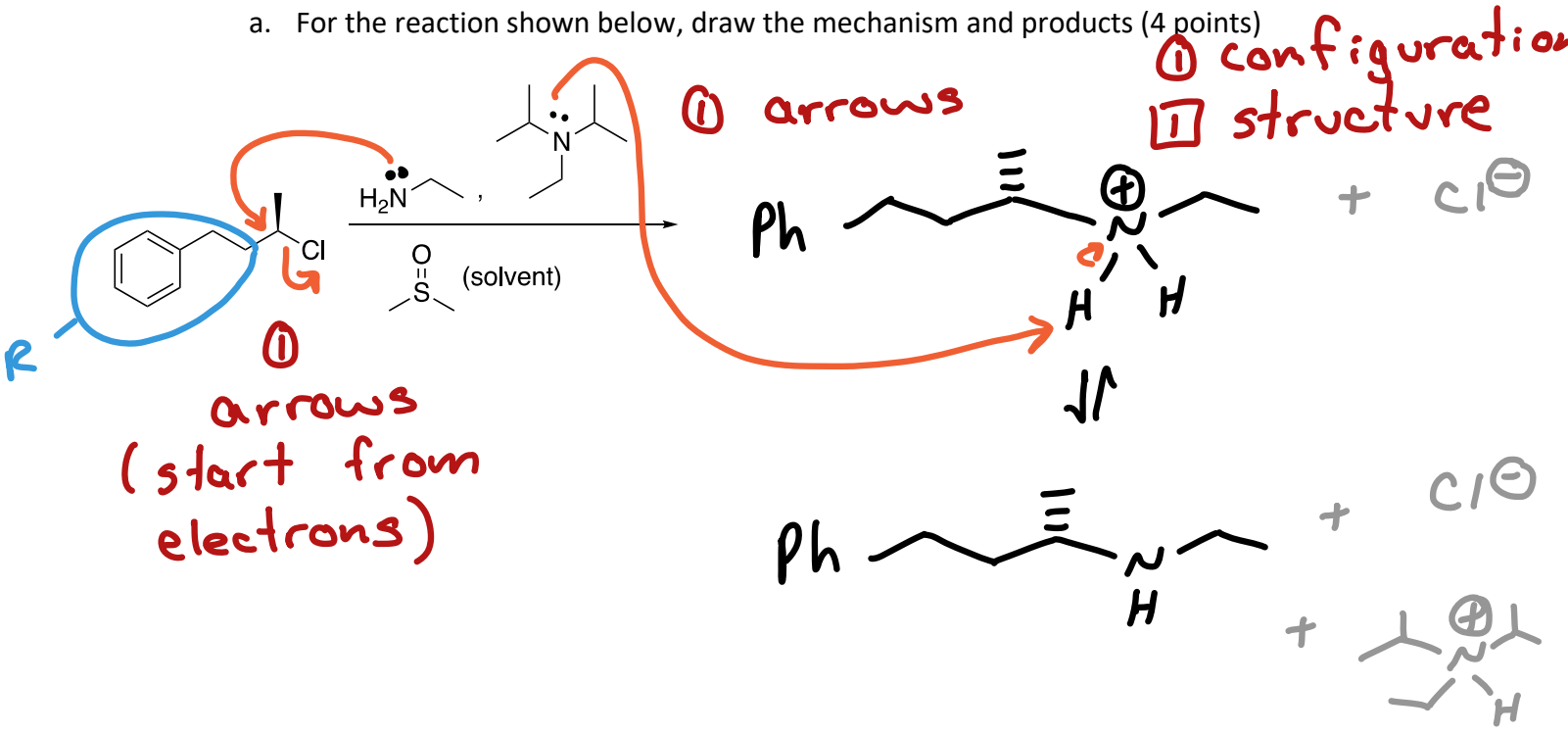
d. In the last step of each mechanism, why is methanol more likely to act as the base than water (linear causal reasoning)? (2 points)

claim → E_a of the RDS is faster.

The methanol is in large ① excess (evidence), which means it is more likely to collide ① with the proton (causal reasoning)

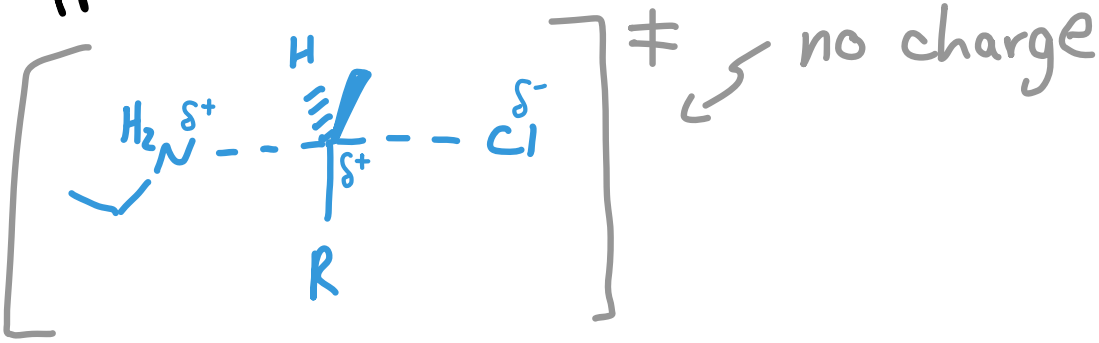
7.

a. For the reaction shown below, draw the mechanism and products (4 points)



b. Draw the transition state structure. (3 points)

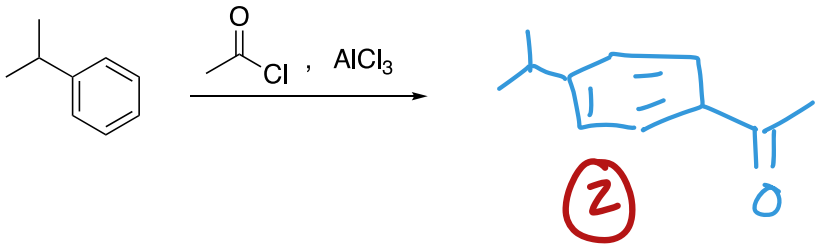
Include partial charges and the overall charge, if applicable



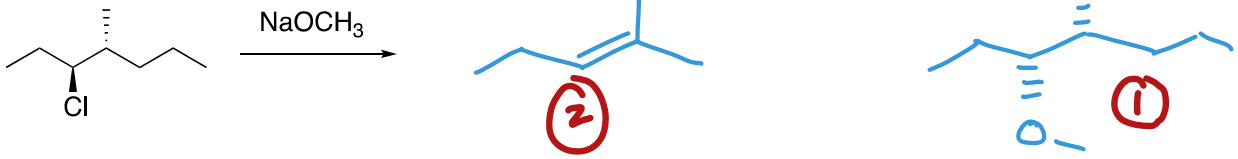
(1) geometry
(1) correct electrophile
(1) partial bonds
(1) partial charges

8. Draw the major organic product(s) for the following reactions. **(2 points each; total 8 points)**

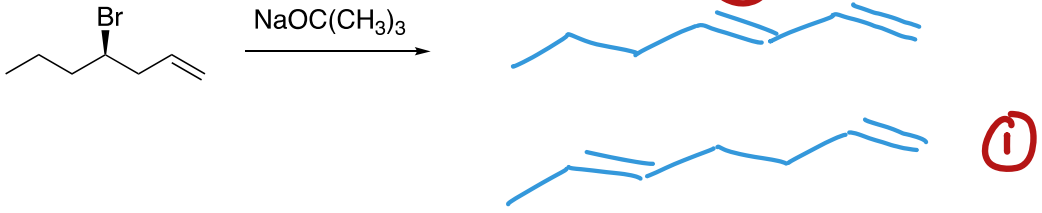
a.



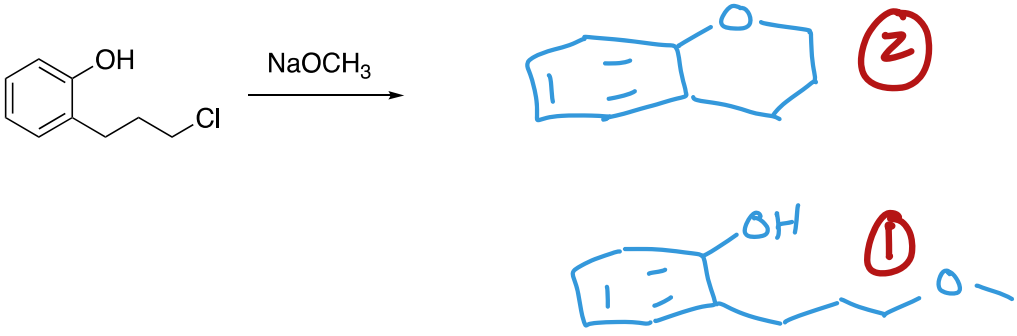
b.



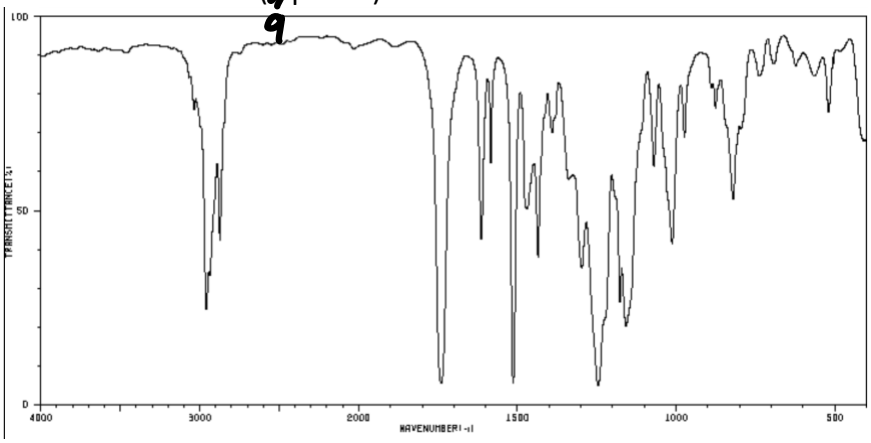
c.

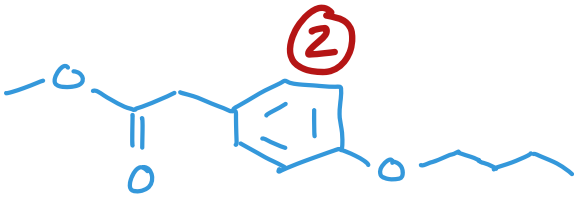


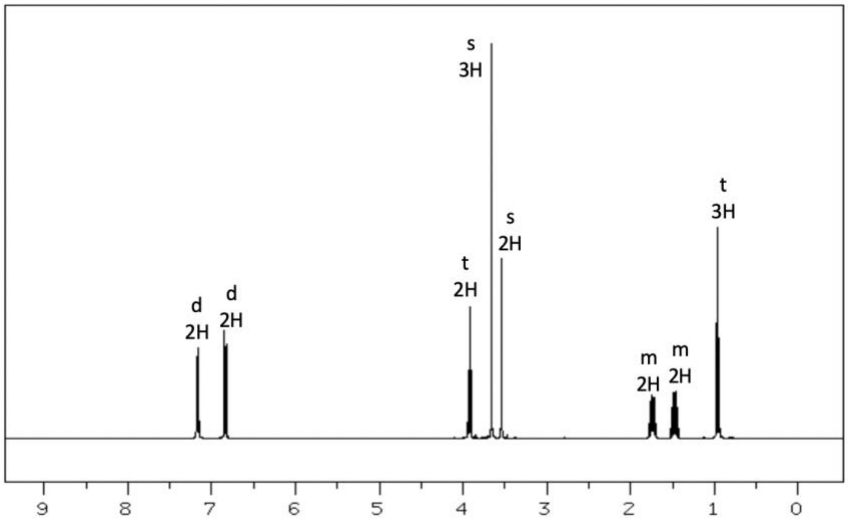
d.



9. Propose a structure that fits the data below. The molecular formula is $C_{13}H_{18}O_3$. You do not have to show your work but part marks will be given for correct fragments if the final structure is incorrect. (9 points)

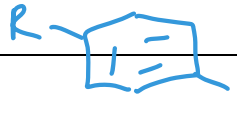






(1) DU = 5

(1) C=O

Peak	Chemical shift	Integration	Multiplicity	Comments/Ideas
A	7.2	2	d	 (1)
B	6.8	2	d	
C	4.0	2	t	OCH_2 next to CH_2 (1)
D	3.6	3	s	OCH_3 (1)
E	3.5	2	s	CH_2 (isolated) (1)
F	1.7	2	m	CH_2
G	1.5	2	m	CH_2
H	1.0	3	t	CH_3 next to CH_2 (1)

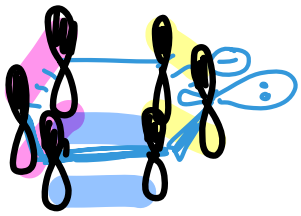
10. What are three online learning skills that are described in the Growth & Goals module (your version). Ideally, these are also ones that you are using or have at least tried. (3 points)

Variety of answers accepted here. Please check back to the G+G module for details.

Bonus

Is the negative charge delocalized in the benzene anion, below? Justify your answer by drawing the relevant molecular orbital(s). (2 points)

no



The electrons are in an (1) sp^2 orbital, perpendicular to the π system. Because the orbitals (1) don't/can't overlap, the lone pair can't be delocalized.