NAME:

Chem 14C
UCLA, Spring 2022
Dr. Ow
Exam 1

Instructions: Write your name at the top of this page. Closed-book and notes. Put away all mobile devices, including smartwatches. Academic dishonesty will not be tolerated. There are six questions over the next four pages. *Students are not allowed to leave early.*

Time limit: 50 minutes.

Circle your TA and section:

Nima Adhami	1F, 1G, 1H	Roberto Chavez	2A, 2D, 2E
Carlos Cruz	1E, 1I, 1L	Vivian Dao	2G, 2H, 2K
Shuaijing Du	1D, 1J, 1K	Ethan Ng	2I, 2J, 2L
Mariah Gomez	1A, 1B, 1C	Zhiyin Yang	2B, 2C, 2F

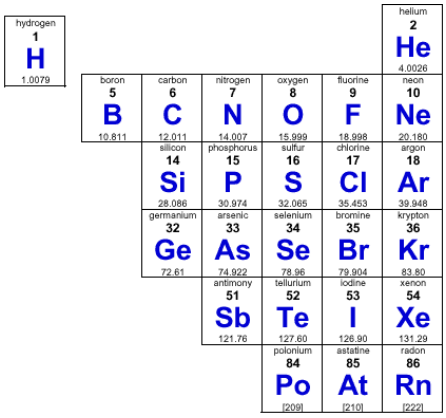

Table 4.3 Change in Free Energy on Flipping from the Cyclohexane Conformer with the Indicated Substituent Equatorial to the Conformer with the Substituent Axial

Substituent	$\Delta G°$ [kcal mol^{-1} (kJ mol^{-1})]	Substituent	$\Delta G°$ [kcal mol^{-1} (kJ mol^{-1})]
H	0 (0)	F	0.25 (1.05)
CH_3	1.70 (7.11)	Cl	0.52 (2.18)
CH_3CH_2	1.75 (7.32)	Br	0.55 (2.30)
$(CH_3)_2CH$	2.20 (9.20)	I	0.46 (1.92)
$(CH_3)_3C$	≃ 5 (21)		
HOC(=O)	1.41 (5.90)	HO	0.94 (3.93)
		CH_3O	0.75 (3.14)
		H_2N	1.4 (5.9)
$CH_3OC(=O)$	1.29 (5.40)		

Increasing size; Increasing $\Delta G°$

Note: In all examples, the more stable conformer is the one in which the substituent is equatorial.

Q1	/10
Q2	/12
Q3	/15
Q4	/12
Q5	/6
Q6	/12
TOTAL	/67

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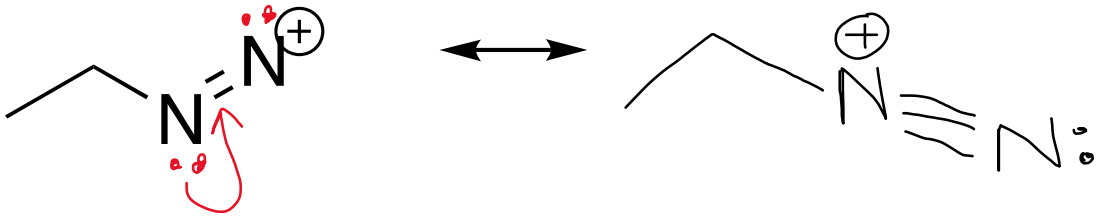
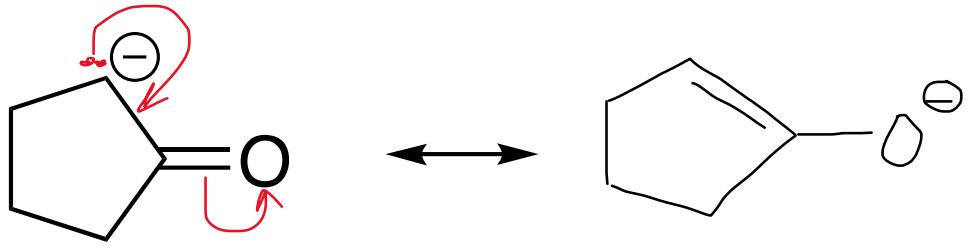
1. Help!!! Each of the following structures is not optimal. Fix them by using curved arrows to show electron movement from the original structure to a better one. Ensure that the new structure you draw is the best one possible. (10 pts)





LEFT SIDE
-1 each incorrectly drawn/missing curved arrow
e.g. arrow is pushed toward negative charge and/or away from positive charge
e.g. sigma bond is pushed
e.g. arrow is pushed toward an sp^3 carbon
-4 pts if no arrows are shown

RIGHT SIDE
-1 each incomplete octet -1 each incorrect/missing formal charge -1 each formal charge of -2/+2
-3 pts each missing structure (no work shown each problem)
THE STRUCTURE DRAWN MUST AGREE WITH THE ARROWS SUPPLIED BY THE STUDENT.
IF NOT, -1 PTS EACH ADDITIONAL ERROR THAT HASN'T BEEN ALREADY DEDUCTED.

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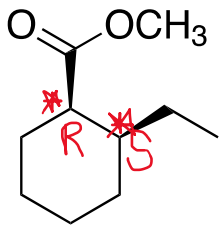
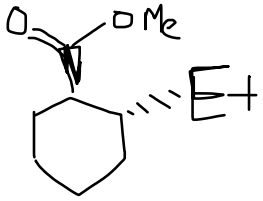
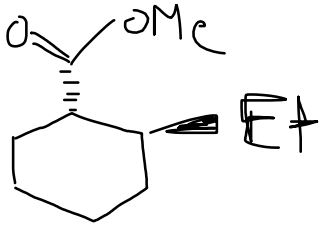
2. Consider the following compound, call it STRUCTURE 1: (12 pts)



a) Write the absolute configuration next to each stereogenic carbon. 4 PTS TOTAL, +2 PTS EACH
(no partial within each one)

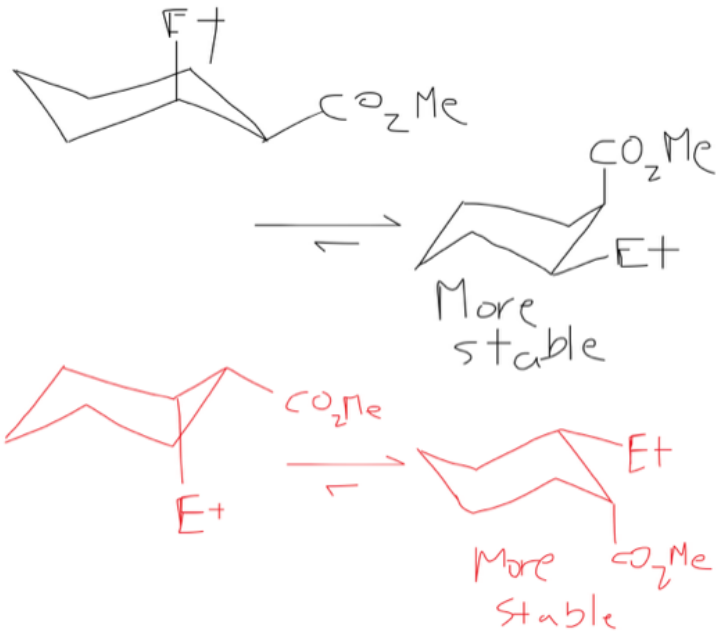
b) Draw all diastereomers of STRUCTURE 1.





4 PTS TOTAL, +2 PTS EACH
IF 2 TRANS AND 1 CIS, THEN 2/4 PTS.
IF 1 TRANS AND 1 CIS, THEN 1/4 PTS.
IF BLANK OR 1 CIS, 0/4 PTS.

c) Draw both chair conformations of STRUCTURE 1. Label which is more stable.



EITHER BLACK OR RED PAIR ACCEPTED.

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4 PTS TOTAL

DEDUCTIONS IF THE TWO CHAIRS ARE NOT CHAIR FLIPS OF EACH OTHER:

-1 PT IF axial doesn't become equatorial and/or equatorial doesn't become axial

-1 PT IF substituent doesn't change from carbon up to carbon down and vice versa

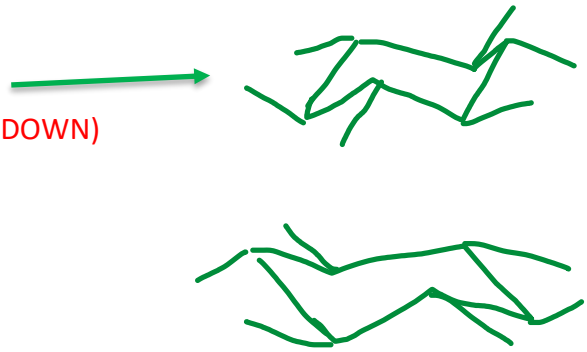
-1 PT DEDUCTION IF MAJOR CHAIR CONFORMATION HAS ETHYL GROUP AXIAL

-1 PT DEDUCTION IF TWO CHAIRS CORRECTLY DRAWN BUT DOES NOT INDICATE WHICH IS MAJOR

-1 PT DEDUCTION IF TRANS CHAIRS ARE DRAWN

-1 PT DEDUCTION IF LOCANTS ARE NOT 1,2

-1 PT DEDUCTION IF ANGLES OF EQUATORIAL GROUPS ARE OFF



-1 PT DEDUCTION IF UP(DOWN) CARBONS DON'T HAVE AXIAL UP(DOWN)

-3 PTS IF ONLY 1 CHAIR CORRECTLY DRAWN

-4 PTS IF BLANK

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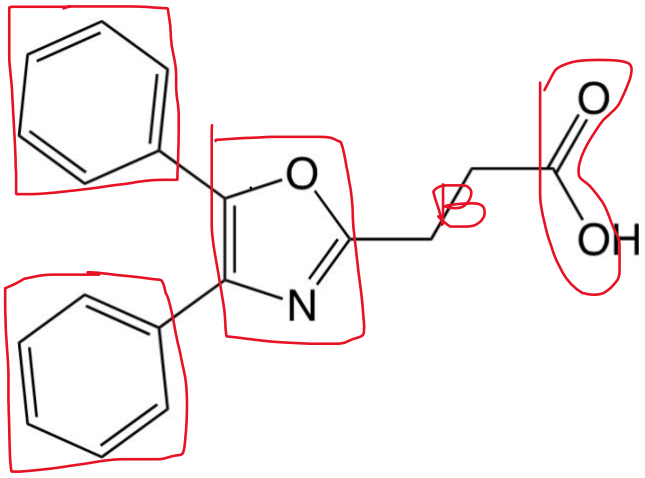
3. Daypro™ (oxaprozin) is a non-steroidal anti-inflammatory drug (NSAID) used to relieve the inflammation, swelling, stiffness, and joint pain associated with osteoarthritis and rheumatoid arthritis. Its structure is shown below. (15 pts)



a) List all functional groups. 5 pts total, -1 pt each missing/incorrect
Benzene (or aromatic), ether (or alkoxy), amine (14D: imine), carboxylic acid (or carboxyl), alkene. In place of ether/amine/alkene, "aromatic" will be accepted.

b) Locate the longest C-C bond. Write "B" (for part b) next to this bond. 1 pt total (no partial)

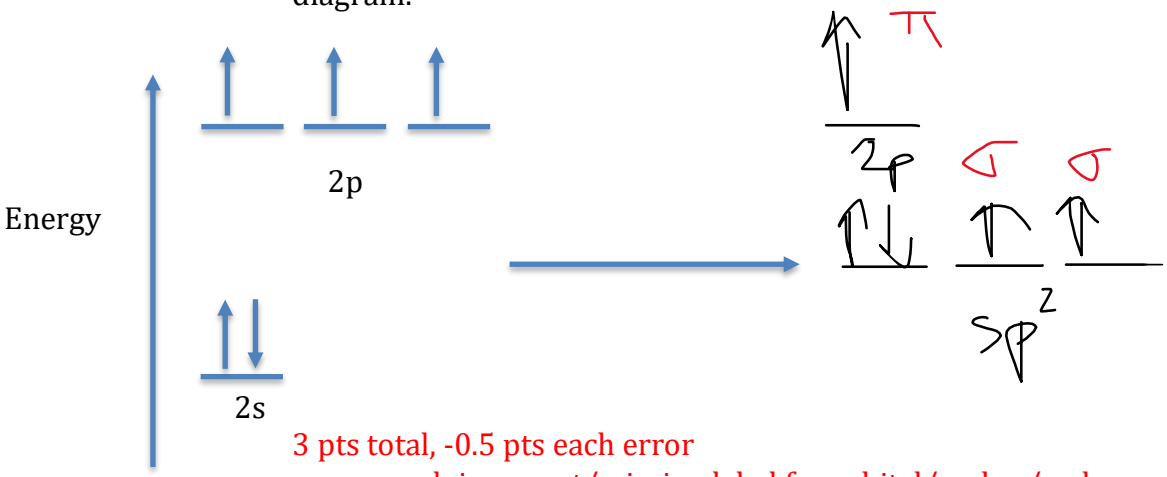
c) Individually BOX each aromatic area. 3 pts total, +1 pt each area

d) CIRCLE each area that is conjugated but not aromatic. 1 pt total, -0.5 pts if proton is circled of -CO_2H group
Will also accept conjugated combinations involving two or more of the aromatic rings
(any 1 of the above = full credit 1/1 pt)

e) How many delocalized π electrons are in the heterocycle? ___**6**____2 pts total(no partial)

f) Complete the hybridization energy level diagram for the nitrogen atom in oxaprozin. The left side has already been completed for your convenience.

- Complete the right side of the diagram, clearly labeling all orbitals.
- Write "σ" or "π" above each unpaired electron located on the right side of the diagram.



3 pts total, -0.5 pts each error
each incorrect/missing label for orbital/σ elec./π elec.
each incorrectly placed/missing electron
automatic 0/3 pts if not sp^2

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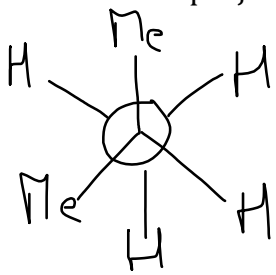
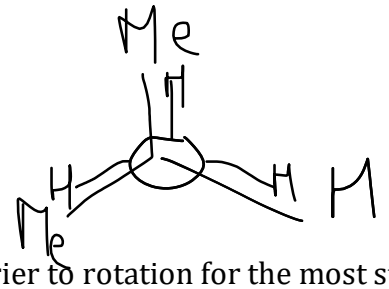
4. Consider 2-methylpropane, looking down the C2-C3 bond. (12 pts)
   a) Draw the most stable Newman projection.



4 pts total, -1 pt each mistake
-4 pts if not staggered

   b) Draw the least stable Newman projection.



4 pts total, -1 pt each mistake
-4 pts if not eclipsed

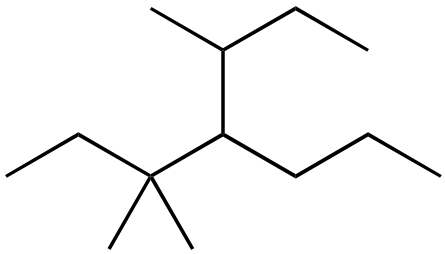
   c) Calculate the barrier to rotation for the most stable conformation rotating to become the least stable conformation. To receive credit, show your work. Use information from the following data:

methyl-methyl eclipsed	2.9 kcal/mol
methyl-hydrogen eclipsed	1.3 kcal/mol
H-H eclipsed	1.0 kcal/mol
methyl-methyl gauche	0.9 kcal/mol

1.3 + 1.3 + 1.0 = 3.6 kcal/mol

4 pts total, -1 pt each mistake
-3 pts if no work shown

5. Name the following compound. (6 pts)



3,3,5-trimethyl-4-propylheptane

-1 pt each error -0.5 pts each missing hyphen, comma
- Incorrect/missing locants
- Parent name (not heptane)
- Substituent names (e.g. no -yl suffix, e.g. not meth- or prop- prefixes)

if 4-sec-butyl-3,3-dimethylheptane or related, then 3/6 pts.
if 3-methyl-4-neopentylheptane or related, then 3/6 pts.

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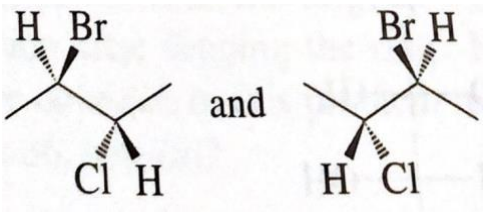
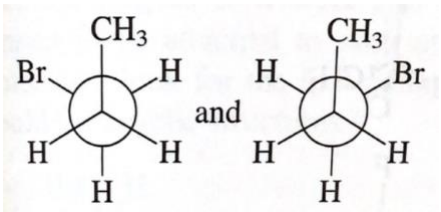
6. For each pair of molecules, indicate whether its members are identical, constitutional isomers, enantiomers, or diastereomers. Write your answer directly below each pair. (12 pts)

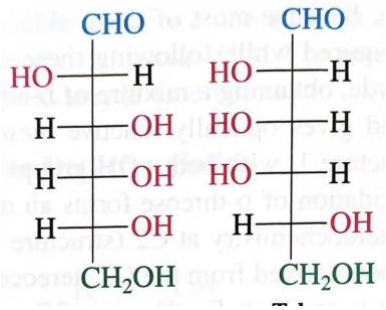
4 pts each, no partial credit within each pair.



enantiomers



identical



diastereomers