CHEM 233, Fall 2018 Midterm #2 Ian R. Gould

COMPLETE THIS SECTION : Up to TWO POINTS will be removed for incorrect/missing information!

PRINTED **FIRST** NAME *Answer Key* PRINTED **LAST** NAME _____

Person on your **LEFT** (or **Empty** or **Aisle**) _____

Person on your **RIGHT** (or **Empty** or **Aisle**) _____

Class you are REGISTERED FOR (onground or hybrid) _____

The room where most students will take the test for your class, i.e. LS A-191 for onground and PS H-152 for hybrid) _____

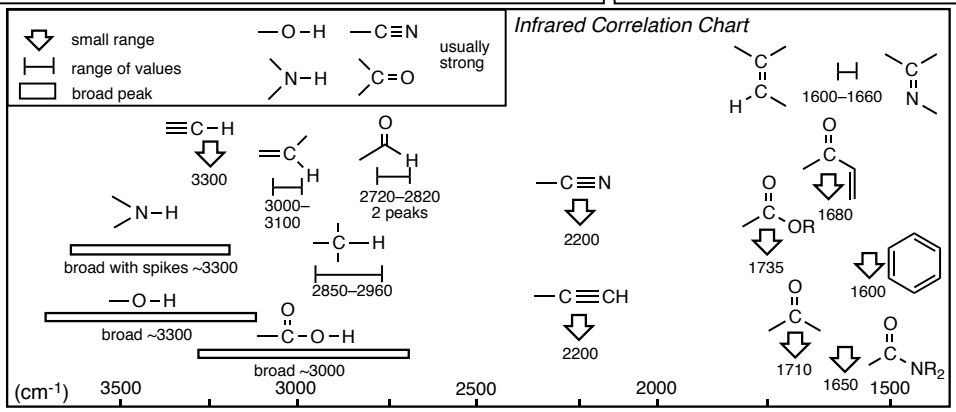
*****YOU ARE NOT ALLOWED TO TAKE SPARE COPIES OF THIS EXAM FROM THE TESTING ROOM*****

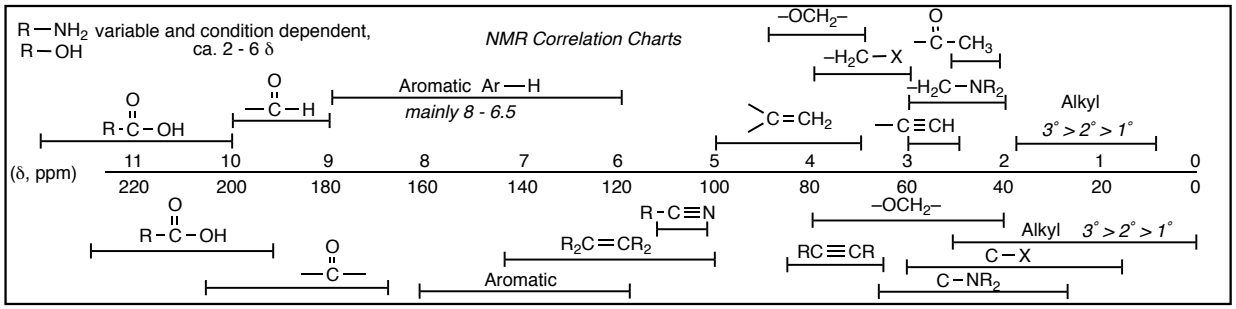
- *PRINT YOUR NAME ON EACH PAGE!*
- *READ THE DIRECTIONS CAREFULLY!*
- *USE BLANK PAGES AS SCRATCH PAPER*
  work on blank pages will not be graded...
- *WRITE CLEARLY!*
- *MOLECULAR MODELS ARE ALLOWED*
- *DO NOT USE RED INK*
- *DON'T CHEAT, USE COMMON SENSE!*

H																	He
Li	Be											B	C	N	O	F	Ne
Na	Mg											Al	Si	P	S	Cl	Ar
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr
Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe
Cs	Ba	Lu	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn

Interaction Energies, kcal/mol

Eclipsing		Gauche	
H/H	~1.0	Me/Me	~0.9
H/Me	~1.4	Et/Me	~0.95
Et/H	~1.8	i-Pr/Me	~1.1
Me/Me	~2.6	t-Bu/Me	~2.7
Et/Me	~2.8		
Et/Et	~3.1		





YOU MUST COMPLETE THIS PAGE WITH YOUR NAME
(EVEN THOUGH YOU ALREADY DID THIS ON THE COVER PAGE)
AND ALSO GIVE YOUR ASU OR POSTING ID NUMBER
WE NEED THIS NUMBER BECAUSE YOU WOULDN'T BELIEVE THE NUMBER OF STUDENTS WHOSE NAMES WE CAN'T READ!

PRINTED **FIRST** NAME **ANSWER** _____ *PRINTED* **LAST** NAME **KEY** _____ *ASU ID or Posting ID* _____

Points by question

1_____**/14**

2_____**/26**

3_____**/26**

4_____**/24**

5_____**/27**

6_____**/34**

7_____**/24**

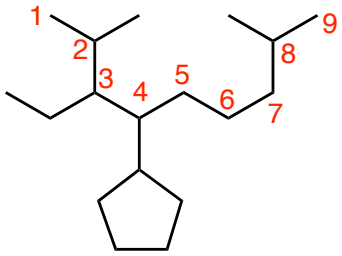
Points Removed for cover errors ____/2

Extra Credit_____/5

Total (incl Extra)_____/175+5

*****YOU ARE NOT ALLOWED TO TAKE SPARE COPIES OF THIS EXAM FROM THE TESTING ROOM*****

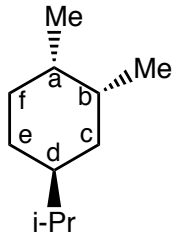
Question 1 (14 pts) Give the IUPAC name for the following structure



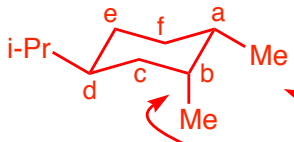
longest chain with max # of substituents

4-cyclopentyl-3-ethyl-2,8-dimethylnonane

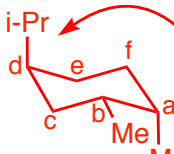
Question 2 (26 pts.)
a) Draw both chair conformations for the provided cyclohexane and calculate the energy difference between the chairs. Indicate CLEARLY which energy factors you are taking into account for each chair. **INDICATE WHICH IS THE LOWEST ENERGY CHAIR**
b) Each carbon in the provided cyclohexane is labelled a, b, c, d etc. Label the carbon atoms on your chairs with the letters a, b, c etc. to identify exactly which carbons in your chairs correspond to which carbons in the provided structure



lowest energy



ΔE = 2.2 kcal/mol



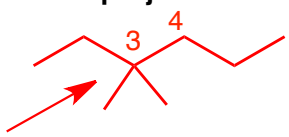
2 x Me/Me gauche interactions here = 1.8
1 x Me/Me gauche interaction here = 0.9
TOTAL = 2.7 kcal/mol

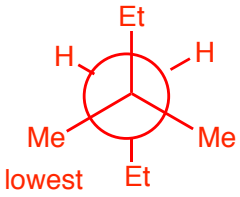
2 x i-Pr/Me gauche interactions here = 2.2
2 x Me/Me gauche interactions = 1.8
1 x Me/Me gauche interaction here = 0.9
TOTAL = 4.9 kcal/mol

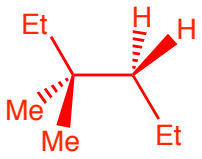
EXTRA CREDIT (5 pts) Which types of structures are the primary constituent of gasoline?

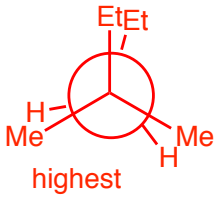
alkenes ketones alkanes aromatics

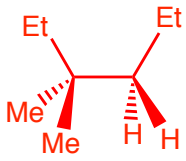
Question 3 (26 pts.) For 3,3-dimethylhexane:
a) Draw a line-angle structure
b) For rotation around the C3-C4 bond, draw Newman projections AND 3D (sawhorse) structures for BOTH the HIGHEST and the LOWEST energy conformations, (clearly indicate which is which). **Your Newman projections should look FROM carbon 3 TO carbon 4.**









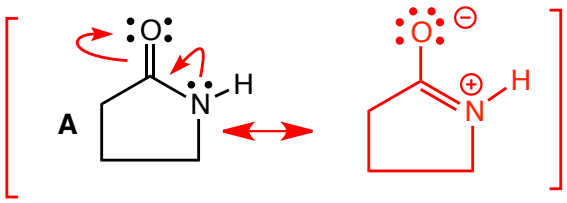


c) Determine the energy difference between these two conformations. CLEARLY indicate the energy factors that you included in your calculation of this energy difference

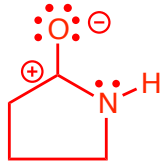
lowest E conformation: 2 Et/Me gauche = 2 x 0.95 = 1.9
Total = 1.9 kcal/mol
highest E conformation: 2 Me/H eclipse = 2 x 1.4 = 2.8
+ 1 Et/Et eclipse = 3.1
Total = 5.9 kcal/mol

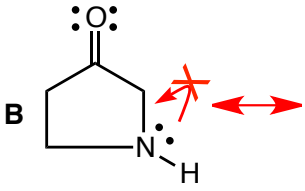
ΔE = 5.9 - 1.9 = 4.0 kcal/mol

Question 4 (24 pts.) The vibration frequencies for the two C=O bonds in **A** and **B** are different. Which would have the higher vibration frequency? Give a brief explanation in terms of **minor resonance contributors** as appropriate. Include drawings of any relevant minor resonance contributors, with all curved arrow pushing, resonance brackets and arrows.

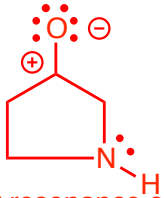


lower frequency





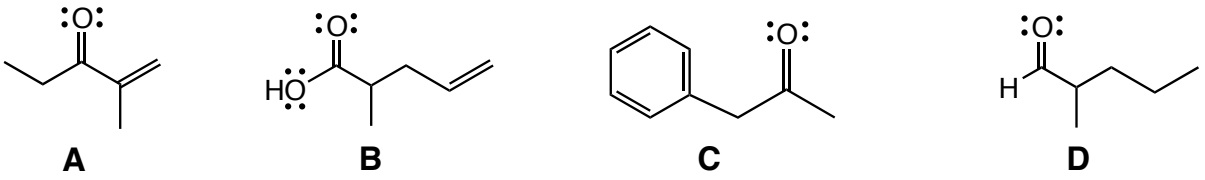
higher frequency
no electron delocalization



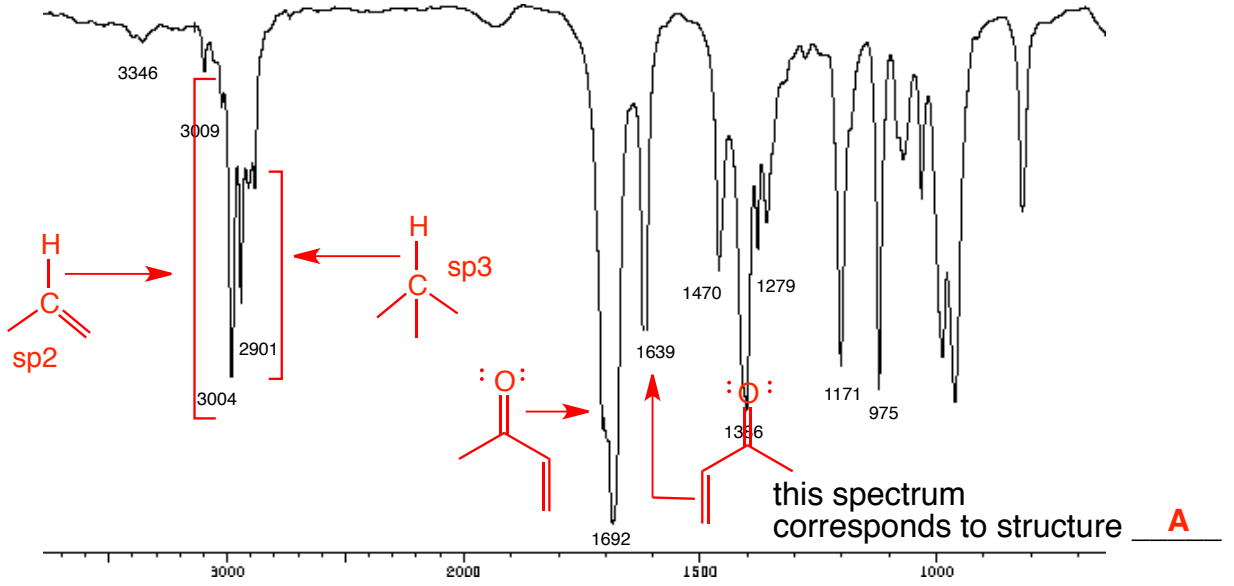
these minor resonance contributors are not wrong, they just don't explain any difference between A and B

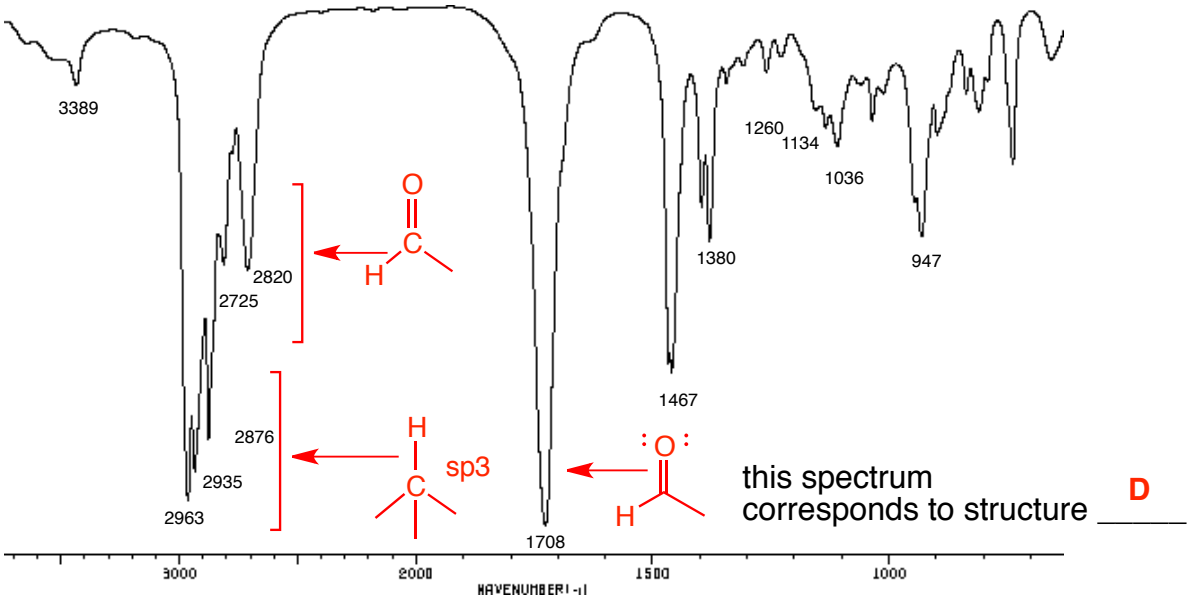
structure A has a minor resonance contributor that has a single C-O bond, AND it contributes more to the resonance mixture than the other minor contributors because it has two formal pi-bonds
structure A has more single bond character in the C=O bond, the C=O bond is thus weaker and vibrates with a lower frequency

Question 5 (27 pts.) Assign the provided IR spectra to ONE of the FOUR provided structures **A** - **D** (two of the structures do not have a provided spectrum). On each spectrum, **identify the peaks that are associated with a specific functional group or type of C-H** bond by **drawing the functional group or bond** and drawing an arrow from **the specific bond in the functional group that vibrates to the absorption peak**.



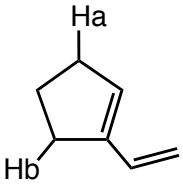
A **B** **C** **D**



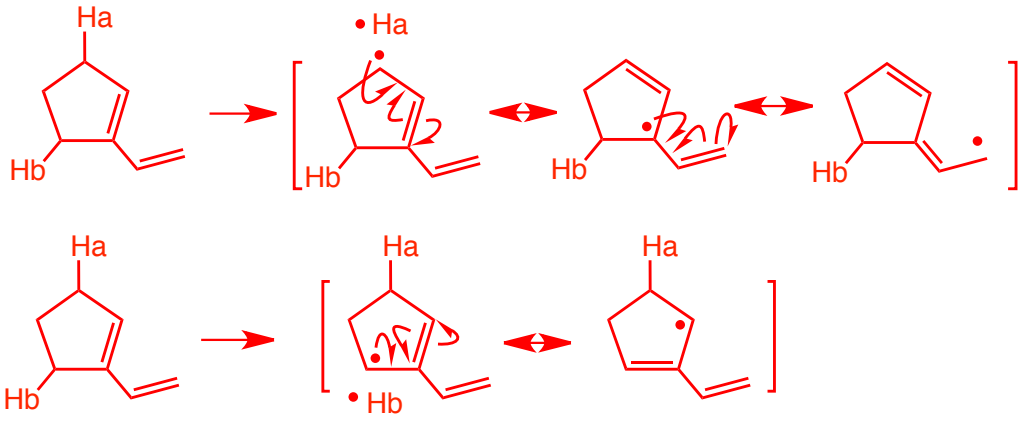


Question 6 (34 pts.)

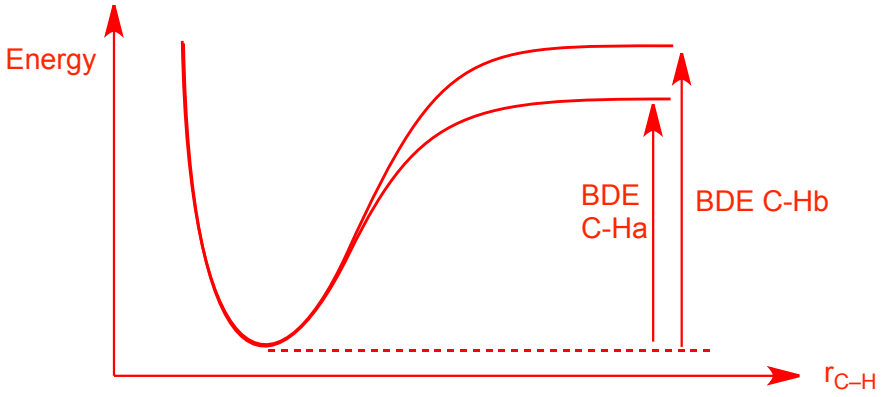
a) Explain which of the bonds C-Ha or C-Hb has the larger homolytic bond dissociation energy. Give an explanation that includes drawings of the products of EACH bond dissociation, including all relevant resonance contributors as appropriate. Include the curved arrow pushing showing how the electron distributions "move" between each contributor and resonance arrows/brackets.



the Ha-C bond has the smaller bond dissociation energy since the radical formed is stabilized by 3 resonance contributors compared to 2 for dissociation of the Hb-C bond



b) Draw an ENERGY DIAGRAM **with properly labelled axes** for cleavage of the C-Ha and C-Hb bonds ON THE SAME DIAGRAM, clearly indicating which diagram refers to which bond cleavage and indicate the MAGNITUDES of the two bond dissociation energies on your diagrams. Deciding where to normalize the diagrams is part of the problem so please don't ask for help with that part.



CHEMISTRY 233, Fall 2018 MIDTERM #2 NAME _____

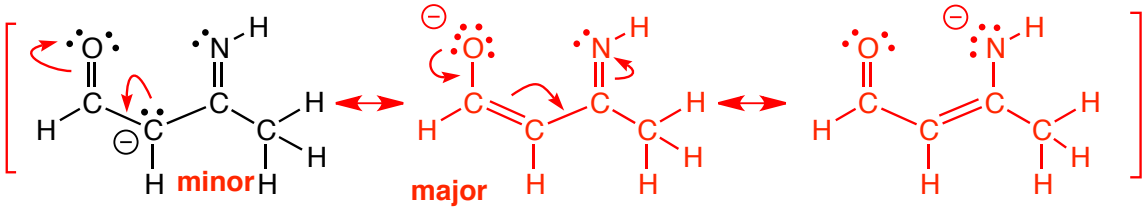
Question 7 (24 pts.) For the following structure:

a) Draw all reasonable resonance contributors, show how they are related using the curved arrow-pushing formalism. Do not forget formal charges and non-bonding electrons as appropriate and resonance arrows and brackets.

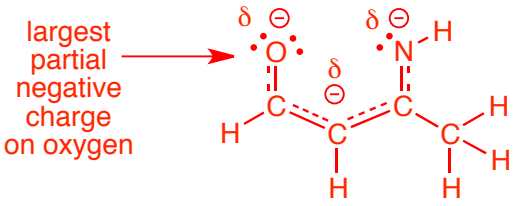
b) Indicate which is the **MAJOR and which is the MINOR** resonance contributor and give a BRIEF explanation for your choices. If there are equal major or minor indicate so.

c) Draw the "actual" resonance hybrid structure using the delta notation to indicate partial charges

d) On your actual structure, indicate which atom will have the LARGEST partial negative charge



the major resonance structure has the formal charge on the most electronegative atom
the minor resonance structure has the formal charge on the least electronegative atom



make sure you answer all FOUR parts of this problem!