CHEM 3311 **HARRINGTON**

Exam 1 7:00 – 8:30 PM February 14, 2017 in HUMN1B50

Instructions. No notes, books, laptops, phones, calculators, models or drawing stencils.

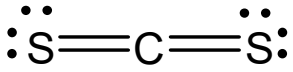
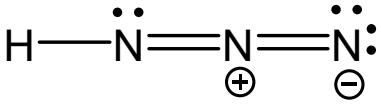
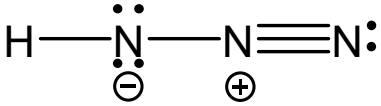
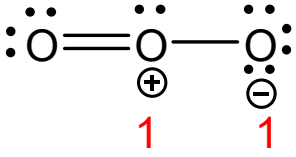
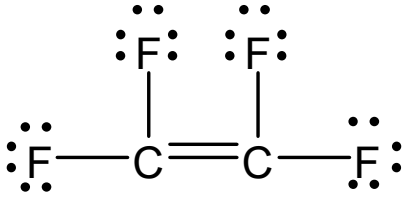
Periodic Table and electronegativity chart are provided.

NAME: KEY version 2 corrected

	Points Possible	Score
1	12	
2	15	
3	16	
4	16	
5	12	
6	16	
7	13	
Exam 1 Total Raw Score	100	
Curve		
Exam 1 Curved Score		
Exam 1 Letter Grade		

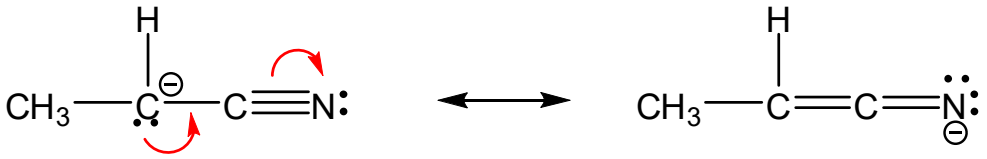
1.(**12 points**) Complete the Lewis Dot structure for each of the molecules below. Calculate the formal charge on each atom in the completed Lewis Dot structure.

NOTE: For molecules which can be represented by resonance hybrids, draw only the most important contributor to the hybrid.

	Formula	**Lewis Dot Structure**	
a.	CS_2		2
b.	HN_3		2
	or		2
c.	O_3		2
d.	C_2F_4		2

2. (**15 points**) For each resonance hybrid provided, draw the two-electron curved arrows that show the conversion of the first contributor to the second. If there is a third contributor, also draw the two-electron curved arrows that show the conversion of the second to the third. Identify the most important contributor to the hybrid and provide a complete evaluation of each contributor to explain why it is the most important.

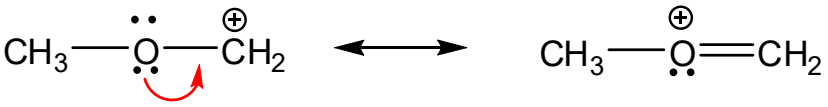
a.



all octets full
9 covalent bonds
(-) on C

most important 1
all octets full
9 covalent bonds
(-) on more electronegative N 2

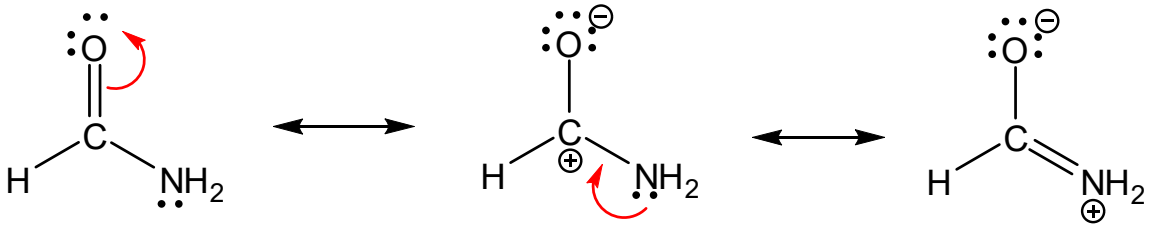
b.



C octet not full
7 covalent bonds

most important 1
all octets full
8 covalent bonds 2

c.



most important 1

all octets full
6 covalent bonds
no (+/-) separation 3
or no formal charges

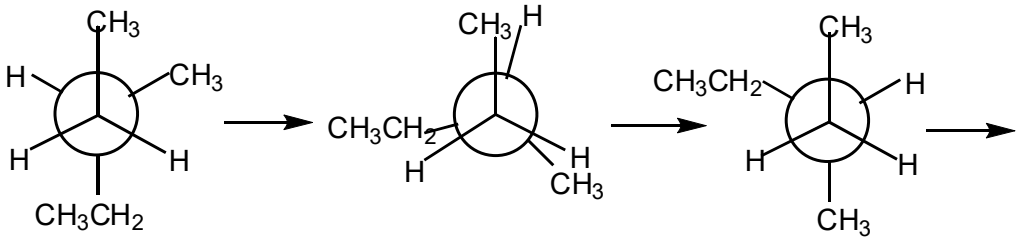
C octet not full
5 covalent bonds
(+/-) separation

all octets full
6 covalent bonds
(+/-) separation

5 arrows 1 point each

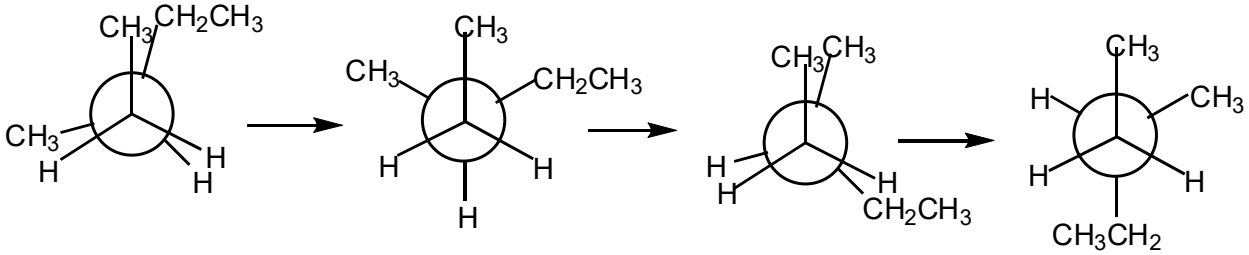
3. (**16 points**) Draw a structure for 3-methylpentane.

Complete the Newman Projections for the conformations of 3-methylpentane obtained by rotation about the C2-C3 bond.
(*Hint*: Rotate the back C 60° clockwise to convert the projection A to B, B to C, etc.)



A **B** **C**

3.3 + 0.4 + 0.4 = 4.1 1
least strain 1



D **E** **F** **A**

11.3 + 5.9 + 3.8 = 21 1
most strain 1

6 projections 2 points each

Use the eclipsing and gauche strain data in the **Tables** below to determine which conformation has the least strain and which conformation has the most strain.

Table 1. Eclipsing Strain Energy (kJ/mol)

	H	**CH_3**	**CH_3CH_2**
H	3.8	5.9	6.3
CH_3	5.9	10.5	11.3
CH_3CH_2	6.3	11.3	13.8

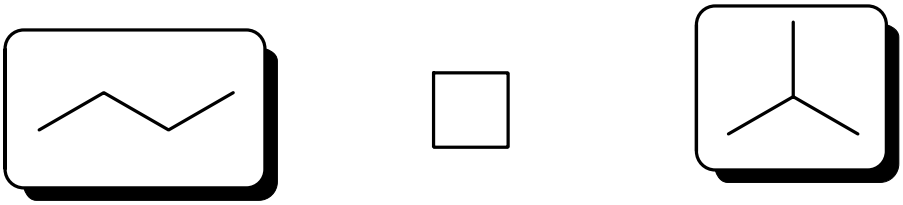
Table 2. Gauche Strain Energy (kJ/mol)

	H	**CH_3**	**CH_3CH_2**
H	0	0	0.4
CH_3	0	3.3	3.8
CH_3CH_2	0.4	3.8	4.6

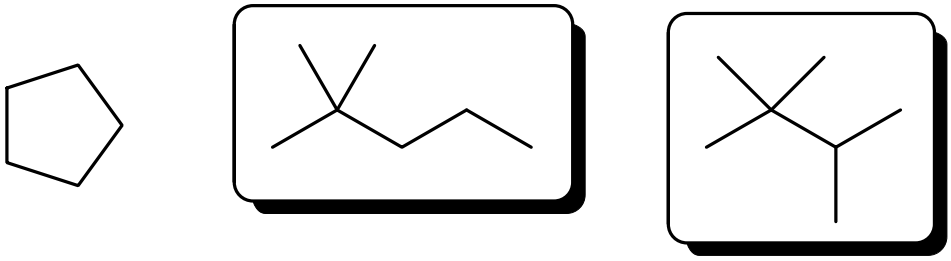
(*For example*: The strain energy associated with an H eclipsing another H is 3.8 kJ/mol.

4. (**16 points**) Draw the structures corresponding to each name.
Which of the compounds in each group are constitutional isomers?

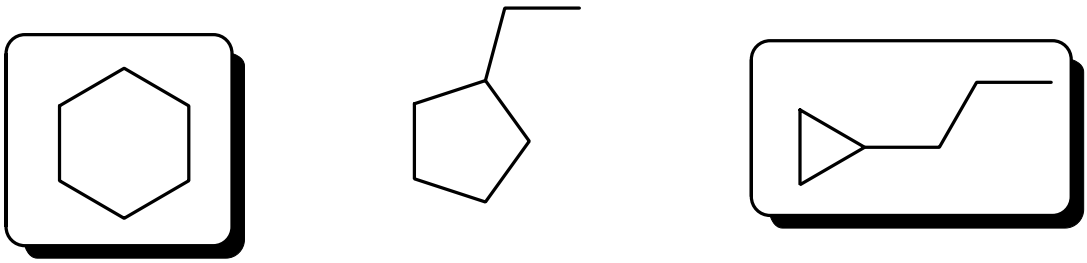
Group 1. butane cyclobutane 2-methylpropane



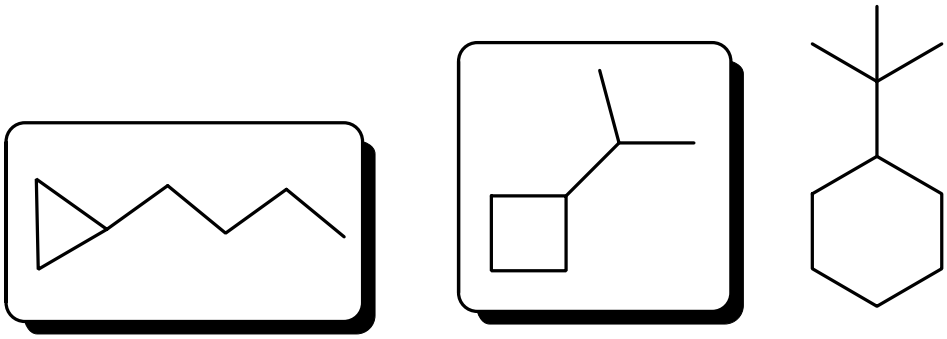
Group 2. cyclopentane 2,2-dimethylpentane 2,2,3-trimethylbutane



Group 3. cyclohexane ethylcyclopentane propylcyclopropane



Group 4. 1-cyclopropylbutane isopropylcyclobutane *tert*-butylcyclohexane



12 structures 1 point each

4 pairs constitutional isomers 1 point each
each incorrect constitutional isomer pairing -1

5. (**12 points**) For each group of three compounds, identify the compound with the highest boiling point and the compound with the lowest boiling point. Explain each answer (identify the intermolecular attractive forces for each compound).

a.

$CH_3(CH_2)_6CH_3$

lowest bp 1

IdId only
lowest surface area

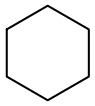
$CH_3(CH_2)_{10}CH_3$

highest bp 1

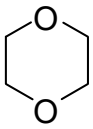
IdId only
highest surface area 2
or more C's in chain

$CH_3(CH_2)_8CH_3$

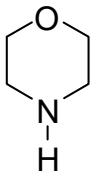
b.



lowest bp 1
IdId only 1

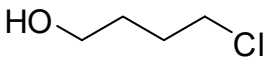


DD
IdId

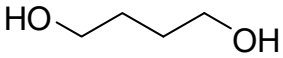


highest bp 1
HB 1
DD
IdId

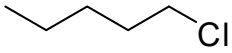
c.



HB (1 donor)
DD
IdId



highest bp 1
HB (2 donors) 1
DD
IdId



lowest bp 1
DD
IdId
NO HB 1

6. (**16 points**) For each set of compounds, identify the most acidic compound and the least acidic compound. Provide an explanation for each answer. Suggested Practice Problem 3.47

a. CH_3CH_2OH Cl_2CHCH_2OH $ClCH_2CH_2OH$

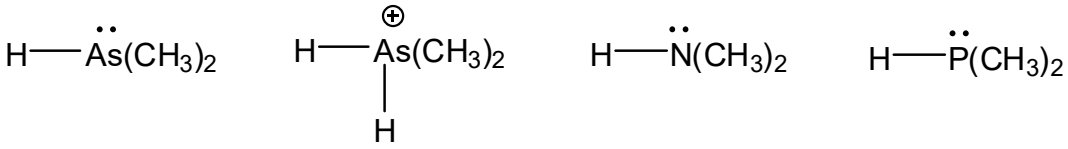
least acidic 1 most acidic 1

Inductive Effect: Cl induces δ+ on attached C. This δ+ stabilizes anion.
Two Cls induce larger δ++ which stabilizes anion more. 2

b. $ClCH_2CH_2SH$ CH_3CH_2OH CH_3CH_2SH

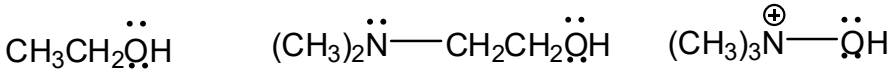
most acidic 1 least acidic 1

Inductive Effect: Cl induces a δ+ on attached C. This δ+ stabilizes anion. 1
Element Effect/size: Anion on large S is more stable than anion on small O. 1

c. 

most acidic 1 least acidic 1

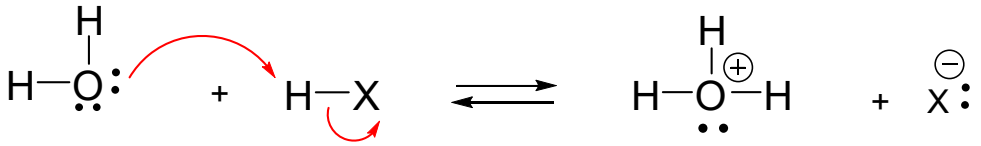
Charge Effect: Conjugate base is a neutral molecule. This is more stable than an anion. 1
Element Effect/size: Anion on smallest N is least stable. 1

d. 

least acidic 1 most acidic 1

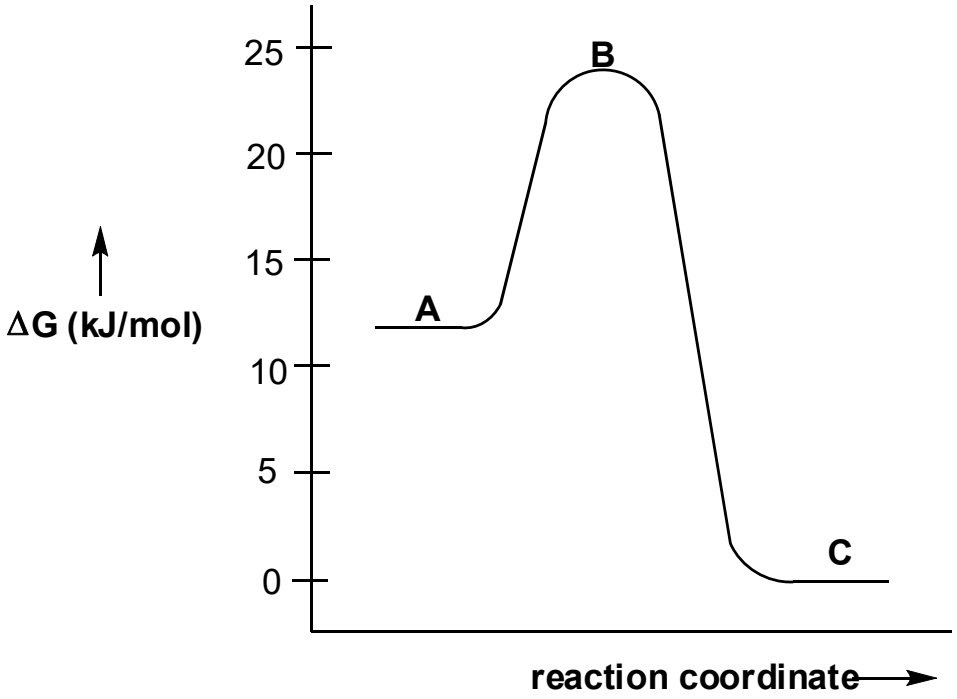
Charge Effect: Conjugate base is a neutral molecule. This is more stable than an anion. or (+)-Charge stabilizes adjacent (-)-charge. 1
Inductive Effect: N induces δ+ on attached C. This δ+ stabilizes anion. 1

7. (**13 points**) For the reaction:



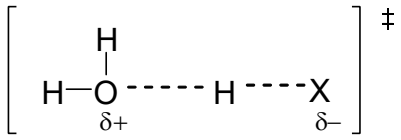
2 arrows 1 point each

Consider the reaction coordinate-energy diagram:



Draw the two-electron curved arrows that show the conversion of reactants to products.

Draw the structure of the reactive species present at point **B** on the diagram.



no linear trajectory -1
no partial charges - 1 each

4 points

Estimate the activation energy (kJ/mol) for the forward reaction. 12 kJ/mol 2

Is the forward reaction endothermic or exothermic? exothermic 2

Estimate the ratio of products to reactants at equilibrium.

ΔG ~ 12 kJ/mol ΔpK$_a$ ~ 2 ratio 100:1 3