

Chem 2210-01 Organic Chemistry

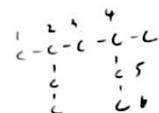
Exam 1

October 16, 2020

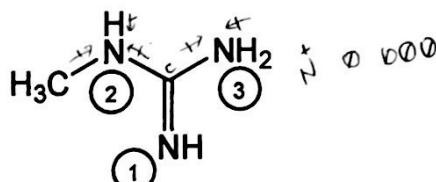
1. The following compound names are all incorrect or incomplete, but they represent real structures. Draw each structure and name it correctly. (8%)

(a) 3-*tert*-butyl-hexane

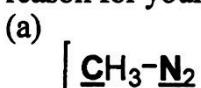
(b) 2,4-diethylpentane



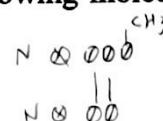
2. The following compound contains three nitrogen atoms. Rank these three nitrogen atoms in an order of decreasing basicity. Give your reason for the arrangement. (5%)



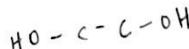
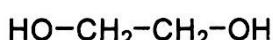
3. What is the hybridization of labeled atom in each of the following molecules. Give a brief reason for your prediction. (12%)



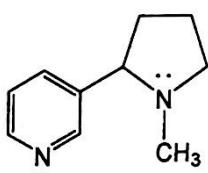
(c)



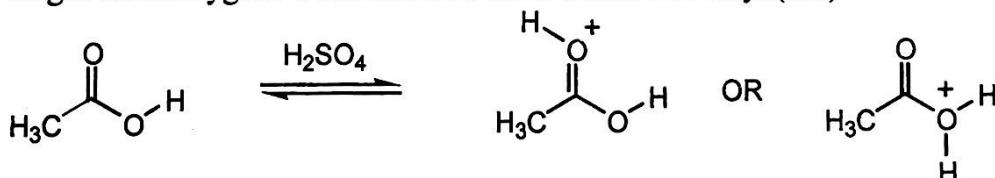
4. Use Newman projection to draw *totally eclipsed*, *eclipsed*, *gauche*, and *anti* conformations for 1,2-ethandiol(ethylene glycol). Which conformer is the most stable one? Give a reason for your prediction. (12%)



5. In which orbitals are the lone pairs in nicotine?(4%)



6. Acetic acid can be protonated by H_2SO_4 either on its double-bond oxygen or on its single-bond oxygen. Which form is more stable and why?(6%)



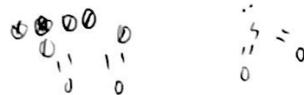
7. Heats of combustion for some alkanes are shown in the following table. What is the strain energy of cyclopropane? (3%)

alkanes	cyclopropane	cyclobutane	cyclohexane	hexane	octane
Heat of combustion (kcal/mol)	499.8	655.9	944.5	995.0	1309.8 163.7

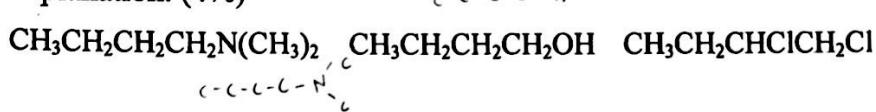
8. A compound has the concentration of 1000 times greater in its acidic form than in its basic form at pH = 6. what is K_a of this compound? (3%)

$$pK_a = \text{pH} + \log \frac{[\text{HA}]}{[\text{A}^-]}$$

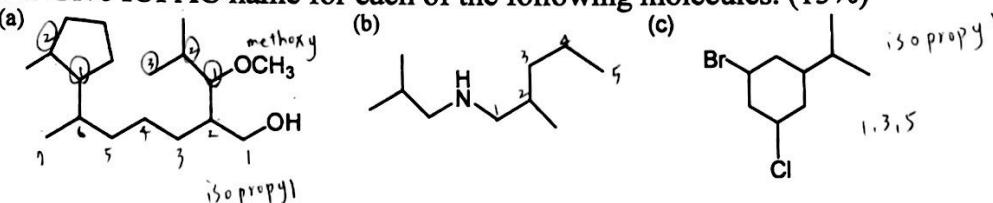
9. Sulfur dioxide has a dipole moment of 1.60 D. Carbon dioxide has a dipole moment of zero, even though C-O bonds are more polar than S-O bonds. Explain this apparent contradiction. (5%)



10. List the following compounds in an order of decreasing boiling point and give a brief explanation. (4%)



11. Give IUPAC name for each of the following molecules. (15%)

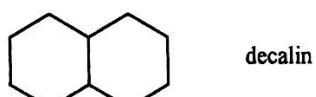


Li Be B C N O F
1 1.5 2 2.5 3 3.5
Na Mg Al Si P S
0.9 1.2 1.5 1.8 2 1.2

12. The energy difference in two chair conformations of *cis*-1,3-dimethylcyclohexane has been measured as about 5.4 kcal/mol. Which is the more stable conformer? (2%) How much of this energy difference is due to the torsional energy of gauche relationships? (Note: One gauche interaction is 0.87 kcal/mol) (4%) And how much energy is due to the additional steric strain of the 1,3-diaxial interaction? (2%)



13. Draw the most stable conformation for each of *cis*- and *trans*-decalin. Use what you know about the conformational energies of substituted cyclohexanes predict which is the more stable isomer. How much energy difference between these two molecules? Give detail information. (10%)

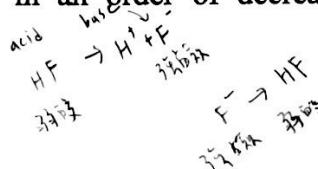


14. Calculate the energy difference between the two chair conformations of *trans*-1,4-dimethylcyclohexane. (5%)
(Note: One gauche interaction is 0.87 kcal/mol)

base $\rightarrow H^-$
acid $\rightarrow H^+$

15. Rank the halide ions (F^- , Cl^- , Br^- , I^-) in an order of decreasing basicity. Give a brief explanation. (6%)

acid $\rightarrow H^+$
base $\rightarrow H^-$
strong \rightarrow weak



記		分			
1	b	2	2		
3	4	4	12		
5	4	6	3		
7	D	8	3		
9	5	10	4		
11	10	12	8		
13	10	14	5		
15	6	16	4		
17		18			
19		20			
總 分		92	4	4	4

國立清華大學試卷

總 分

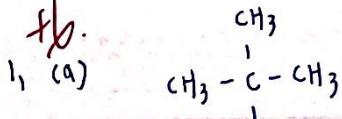
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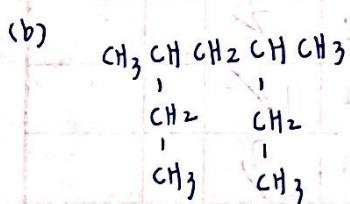
學 號 108023025

姓名 張小宣

日期 109,10,16



3-ethyl-2,2-dimethylhexane



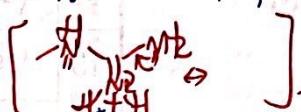
2-ethyl-4-methylhexane

3,5-dimethylheptane

~~2, + basicity ① > ② > ③ #~~

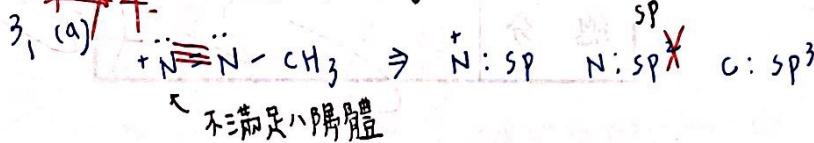
~~N① sp² hybridization, more %s than sp³, bonding electrons closer to nucleus, most stable (weak)~~

For conjugated acid,



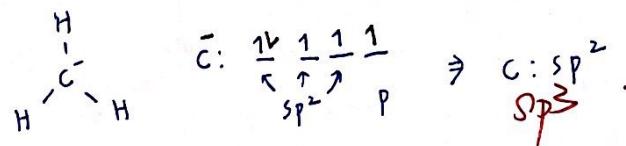
~~N③ bonds with more H (RNH₂ pKa ~ 10), strongest conjugated acid~~

~~stronger the conjugated acid, weaker the basic inductive effect~~

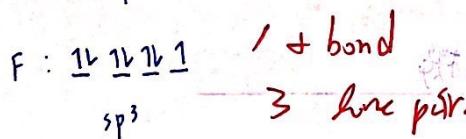
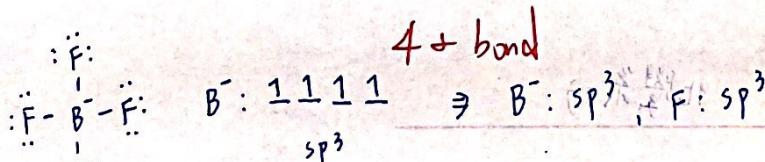


~~N: 1L 111
N: 1L 111
C: 1 111~~

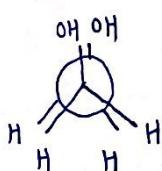
(b)



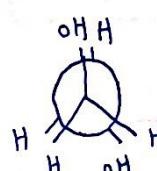
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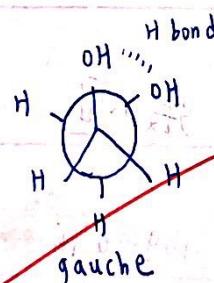
+1/2



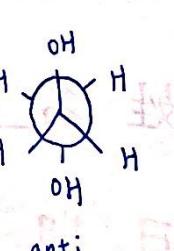
totally eclipsed



eclipsed



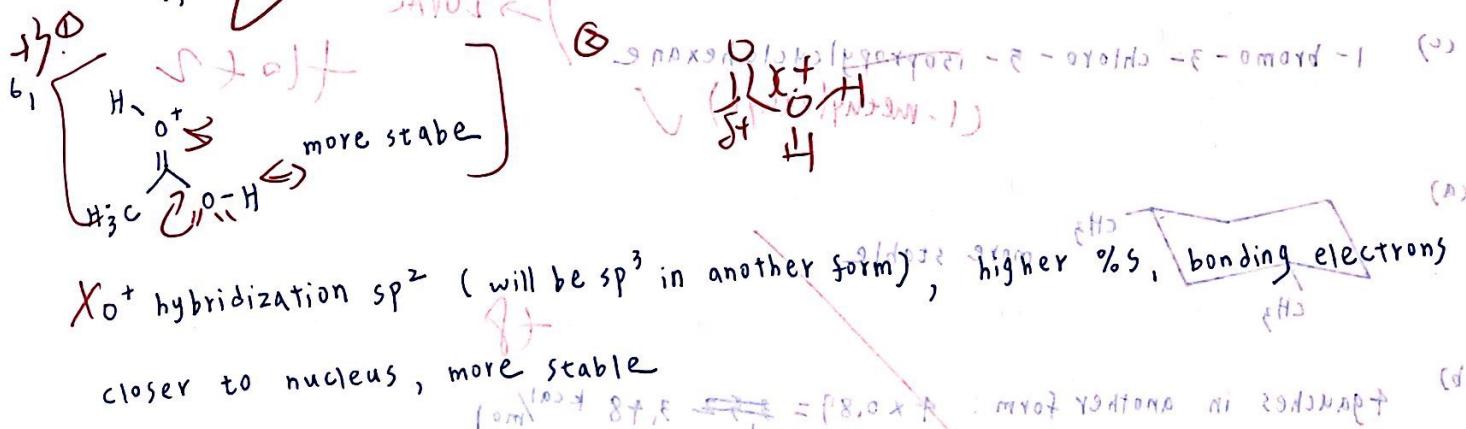
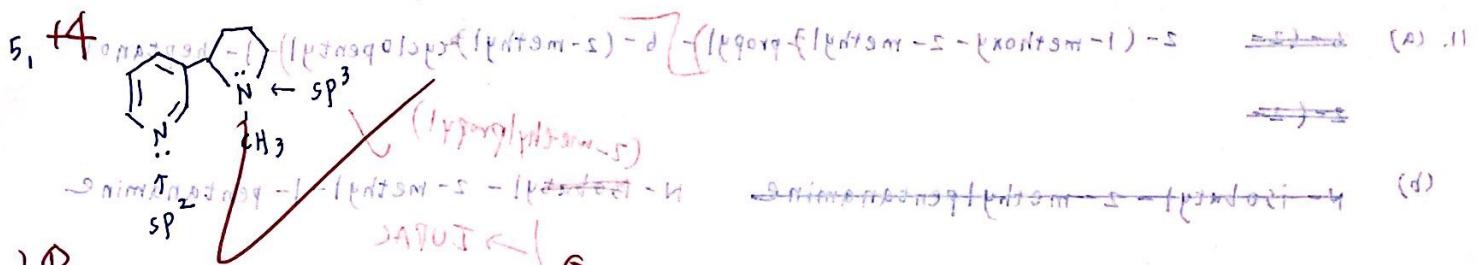
gauche



anti

gauche most stable #

stagger is more stable than eclipse, while there is H bond in gauche conformation



Heat of combustion of propane (X) $\frac{6-3}{8-6} = \frac{995-X}{1309.8-995}$ $X = 522.8 \text{ kcal/mol}$

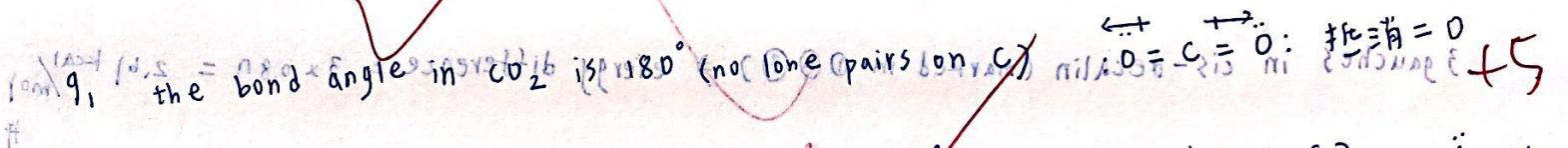
$$\Rightarrow \text{strain energy} : = 522.8 - 499.8 = 23 \text{ kcal/mol}$$

$$\frac{1309.8 - 995.0}{2} = 157.4 \text{ (CH}_2\text{)}$$

$$499.8 - 444.7 = 55.1 \quad 157.4 \times 3 = 472.2 \quad 499.8 - 472.2 = 27.6$$

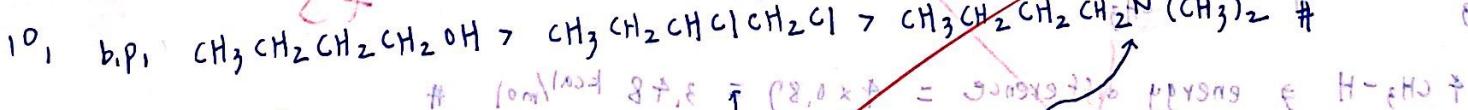
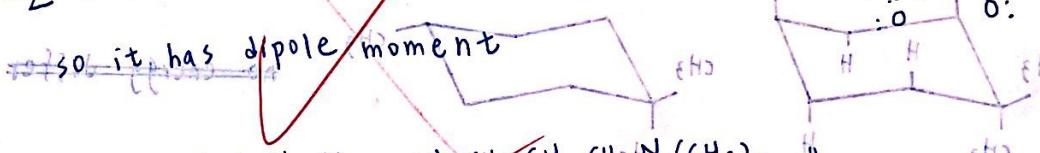
$$499.8 - 3 \left(\frac{995.0}{6} \right)$$

8, $pK_a = 6 + \log \frac{1000}{1}$, $pK_a = 9$, $K_a = 10^{-9} \text{ (M)}$



while bond angle in SO_2 is smaller than 180° (one lone pairs on S)

~~so it has dipole moment~~



can form hydrogen bond

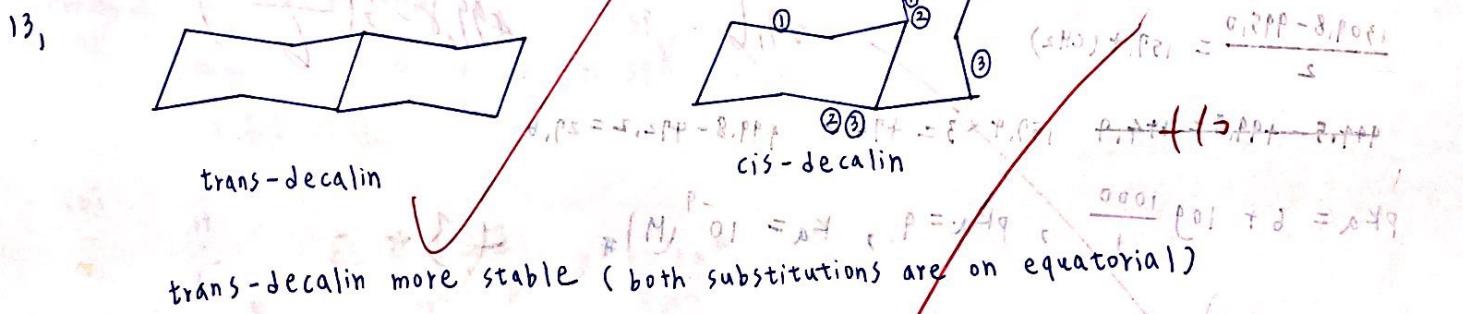
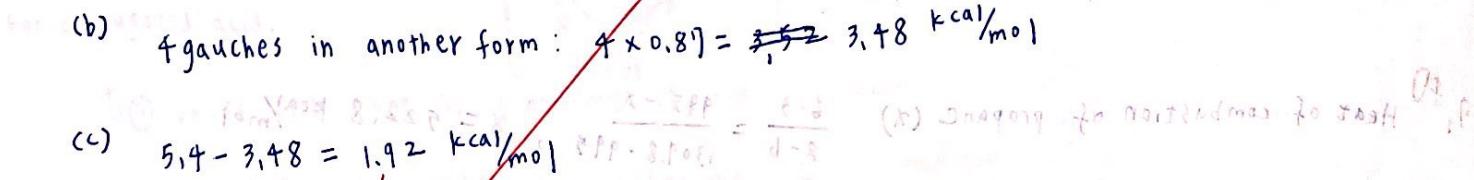
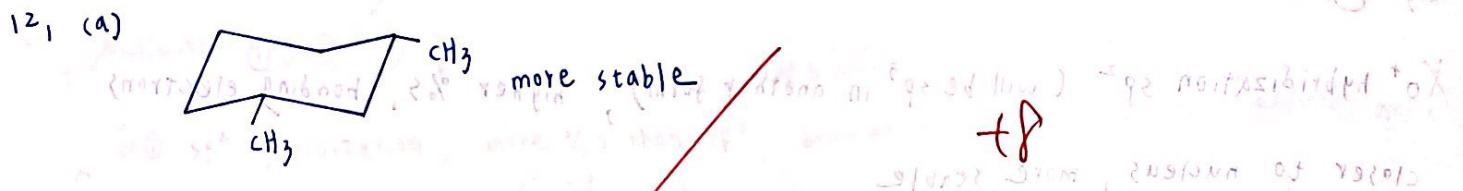
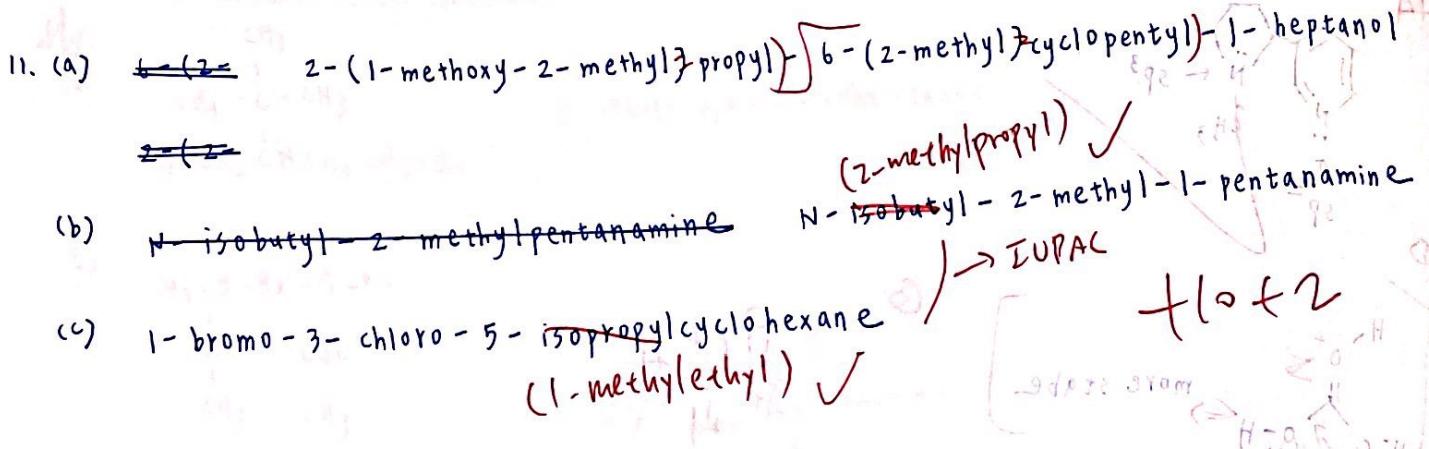
(strongest non-covalent interaction)

larger dipole (2Cl vs. 1N),

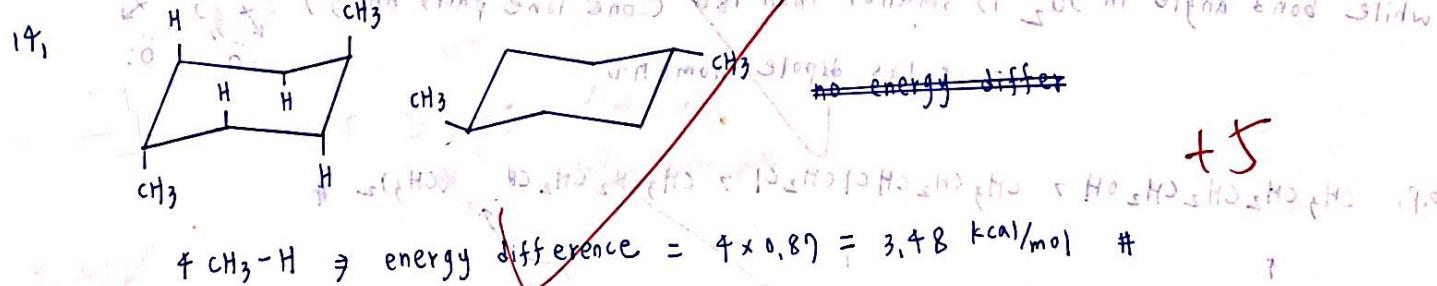
& doesn't have H_2O London force also bigger

~~it's not polarized~~ \leftrightarrow ~~less strong~~ \leftrightarrow ~~less strong~~

~~attraction~~ \leftrightarrow ~~attraction~~ \leftrightarrow $\text{IH} < \text{RH} < \text{DHF} < \text{THF}$



3 gauches in cis-decalin (marked in ① ② ③) \Rightarrow energy difference $= 3 \times 0.87 = 2.61 \text{ kcal/mol}$



15. conjugated acid: HF, HCl, HBr, HI
 bigger the size, lower the electron density (more stable) \Rightarrow HI weakest conjugated acid
 strong basic has weak conjugated acid \Rightarrow basicity $\text{I}^- > \text{Br}^- > \text{Cl}^- > \text{F}^-$

pKa HF > HCl > HBr > HI (\rightarrow electron density \downarrow)

\uparrow conjugated
 strongest acid, weakest conjugated base

\Rightarrow basicity $\text{F}^- > \text{Cl}^- > \text{Br}^- > \text{I}^-$

+6