6

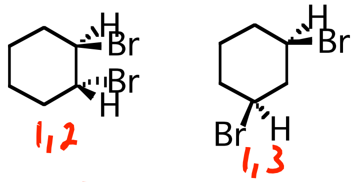
Answers, Test 1 Version 3

JASPERSE CHEM 350 TEST 1 VERSION 3 Organic Chemistry I - Jasperse
Intro and Review
Structure and Properties of Organic Molecules
Structure, Nomenclature, and Conformation/Stereochemistry of Alkanes

1. (12 points) Give the relationship between the following pairs of structures. The possible relationships are the following:

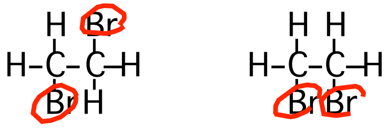
same compound	structural isomers	resonance structures
stereo isomers	not isomers (different molecular formula)	

a.



Structural.
1,2-dibromo vs
1,3-dibromo.

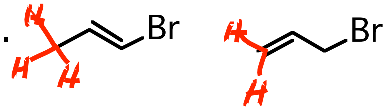
b.



Same.
Bond rotation around single bonds is allowed.

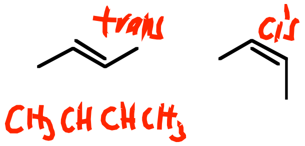
1. Resonance: No atoms can move!
2. Stereo: same condensed formula
3. Structural: different condensed formula

c.



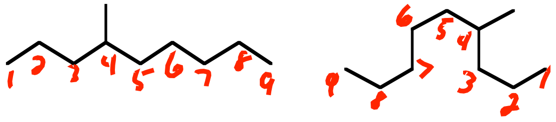
Structural
CH3CHCHBr vs CH2CHCH2Br

d.



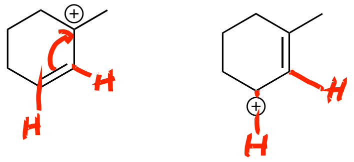
Stereo Trans-cis.
Double bond can't rotate.

e.



Same. Both are 4-methylnonane

f.



Resonance. Electrons and charge is repositioned, but no atoms moved.

2. (8 points) Draw line-angle structures and names for 4 of the 5 structural isomers of C_6H_{14}. → acyclic

Alkane Acyclic: C_nH_{2n+2}
Alkane Cyclic: C_nH_{2n}

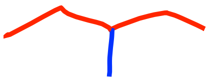
Beware of drawing same thing twice!

6

hexane

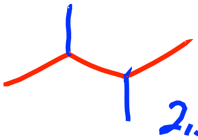
5

2-methylpentane

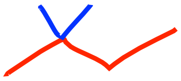


3-methylpentane

4

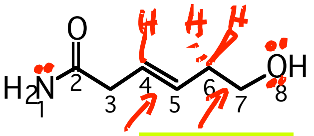


2,3-dimethyl butane



2,2-dimethylbutane

2,3-dimethylbutane



3. (10 Points)
a. For the above structure, what is the hybridization and approximate bond angles (109, 120, or 180) about:

C-2 sp2, ~120°, trigonal planar

C-4 sp2, ~120° trig planar

C-6 sp3, ~109 tetrahedral

O-8 sp3, ~109 tetrahedral

b. In the above structure, N-1 is actually found to have 120° bond angles. (This may seem unexpected to you at this point, but we'll learn why later in the course.) What must be the hybridization of the nitrogen?

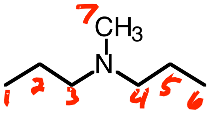
sp2. Hybridization, bond angle, and electron geometry are all interlocked. To know any one of them is to know the others.

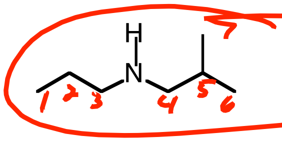
4. (2 Points) Bond rotation around C6-C7 in the above structure has a 7 kcal/mol barrier, while rotation around the C4-C5 bond has a 70 kcal/mol barrier. Explain very briefly why it is so much harder to rotate the latter bond?

Single bond versus double bond.
A double bond has overlapping p-orbitals.
To rotate a double bond, the p-p overlap would be lost. The full pi-bond would need to break.
By contrast, no bonds are broken when you rotate around a single bond.

5. (4 points) For each of the pairs listed, circle the one with the higher boiling point.

a.

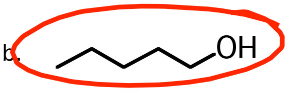


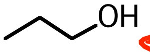


H-bonding

2 factors:
1. H-bonding (raises ~~solubility~~ bp.)
2. London force (# of carbons)
-more C's ~~reduces~~ water solubility raises bp

b.



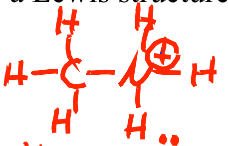


Extra carbons, hydrophobic

more water soluble

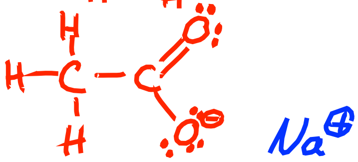
6. (6 points) Write a Lewis structure and assign any non-zero formal charges.

a. $[CH_3NH_3]^+$

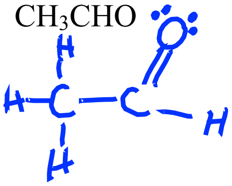


1. Want normal bonding for all: in absence of metal ions
2. C=O (or C=C in other cases) may help
3. If you have any formal charges ([redacted]), they must sum to net charge of molecule (zero, in this case)
4. Organization must match condensed formula sequence

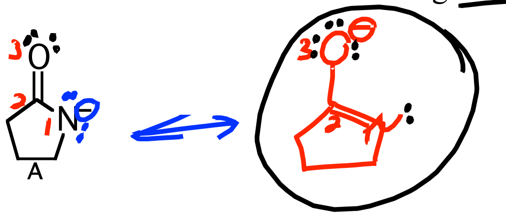
b. CH_3CO_2Na ⊖ ⊕



c. CH_3CHO



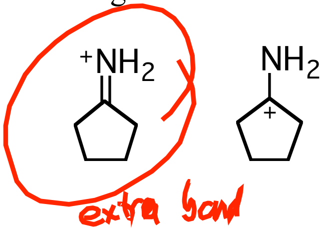
7. (5 points) a) Draw the best resonance structure for anion A, and circle the resonance structure that would make the greater contribution to the resonance hybrid.



$C^{\ominus}$ $N^{\ominus}$ $O^{\ominus}$ $\xrightarrow[\text{eneg}]{}$

2 Factors:
1. More bonds (priority)
2. Electronegativity (if bonds are equal)

b. For the two resonance structures shown below, circle the resonance structure that would make the greater contribution to the resonance hybrid.



extra bond

8. (6 points) Rank the acidity of the following molecules, 1 being most acidic, 4 being least acidic. Hint: draw the anions!

C N O X $\xrightarrow{\text{eneg}}$ $\xrightarrow{\text{anion stability}}$

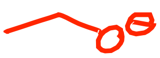
Think Anion

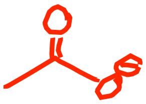
NH_3 4 CH_3CH_2OH 3 CH_3CO_2H 2 HCl ①

3 Acidity Factors:
1. ✓ charge (not relevant here)
2. Eneg
3. Resonance

$^{\ominus}NH_2$

least stable



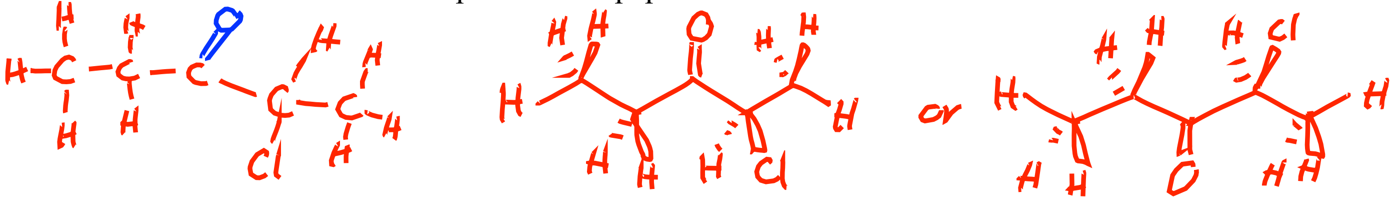


resonance

$Cl^{\ominus}$

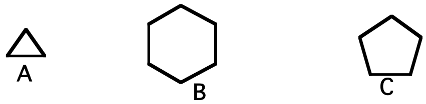
most stable

9. (6 points) Draw a line-angle picture for all of the atoms in the molecule $CH_3CH_2COCHClCH_3$, including the hydrogens. Use the hash-wedge convention to indicate atoms that are not in the plane of the paper.



Cl could equally well be drawn in the hashed spot

10. (5 points) Rank the ring strain in the following, from 1(most) to 3 (least). Explain very briefly the differences in strain.



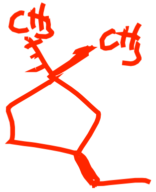
A	B	C
1	3	2

A: has large angle strain (60° angles, not 109° angles)
B: By taking on chair conformation, there is zero angle strain, and zero torsional (no eclipsing)
C: If it has ideal angles, then some eclipsing and torsional strain destabilizes it

T

11. (6 points) Which of the following are capable of cis-trans stereoisomerism? (Yes/No).

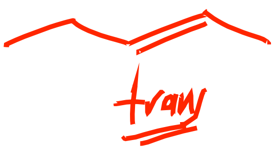
a. 3-ethyl-1,1-dimethylcyclopentane

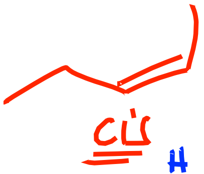


No

no cis/trans distinction

b. ~~3~~ 2-pentene (name means a double bond is between carbons 3 and 4)





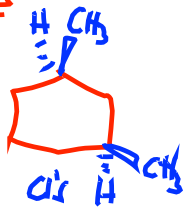
Yes

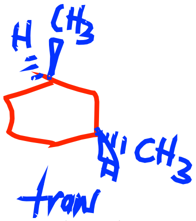
cis/trans

c. 1,3-dimethylcyclohexane

Yes

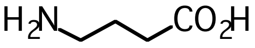
cis/trans





T

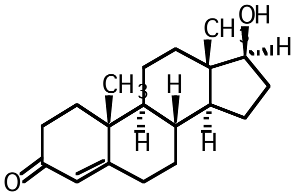
12. (9 points) Identify the functional groups in the following molecules. (Do not include "alkane", since that is not "functional". And do not specify "cyclic".)

a. 

("GABA: brain neurotransmit

Amine

Carboxylic Acid

b. 

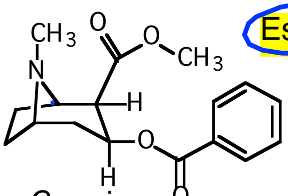
Testosterone

Alcohol

Ketone

Alkene

T

c. 

Cocaine

Ester

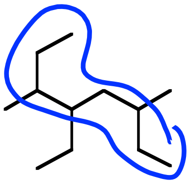
Arene or aromatic

Amine

Ester

13. (5 points) Give the IUPAC name for the following compounds.

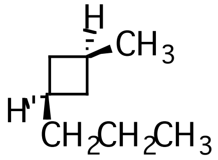
a.



1. Longest chain
2. Alphabetize substituents
3. Number from end near substituent

4-ethyl-3,6-dimethyloctane

b.

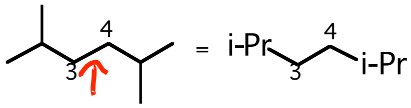


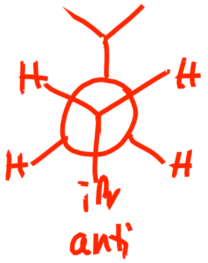
1. cis/trans for di-subbed rings
2. Alphabetize substituents
3. Numbering
4. Know isopropyl and t-butyl

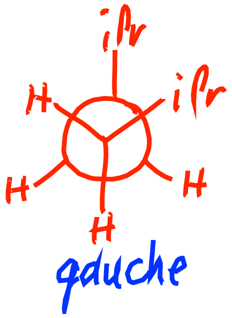
cis-1-methyl-3-propylcyclobutane
or
cis-3-methyl-1-propylcyclobutane

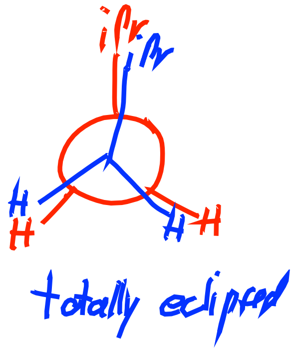
14. (8 points) a. Draw Newman projections for the totally eclipsed, the gauch, and the anti conformations of 2,5-dimethylhexane, relative to the C3-C4 bond. You may abbreviate the isopropyl groups attached to C3 and C4 as "i-Pr" for convenience.

b. Explain very briefly why the rotation barrier around the C3-C4 bond of 2,5-dimethylhexane is greater than the rotation barrier in butane.







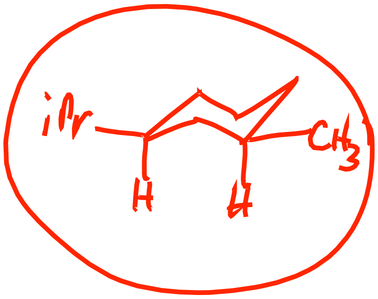


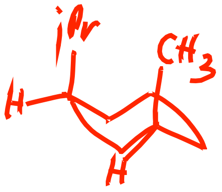
b. Steric Strain. Larger rotation barrier because greater steric strain in total eclipse between two larger isopropyl groups compared to steric strain between two methyl groups. Torsional stain is common to both, to the difference is the difference in steric strain.

15. (8 points) a.) Draw the two chair conformations of cis-1-isopropyl-3-methylcyclohexane. (You don't need to show the H's on carbons other than 1 and 3). For convenience, you may abbreviate methyl as "Me" and isopropyl as "iPr"

b.) Circle the more stable conformation.

c) Would trans-1-isopropyl-3-methylcyclohexane be more stable or less stable than the cis isomer?





1. Make sure you've really drawn "flipped" chairs
2. What's "ax" in one chair flip is "eq" in the other.
3. Process cis-trans
4. Draw in H's on substituted carbons (easier to see ax/eq).