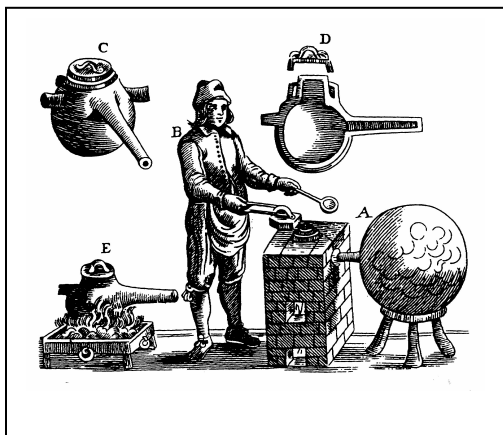




Chemistry

107 A

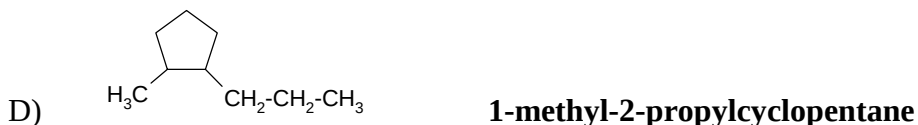
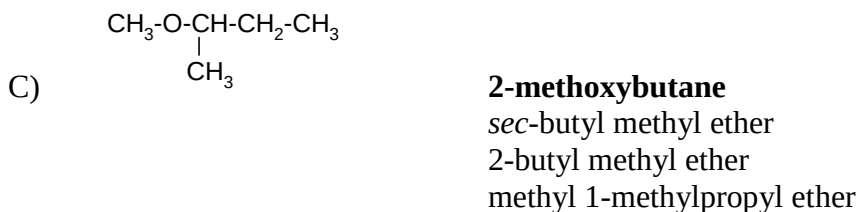
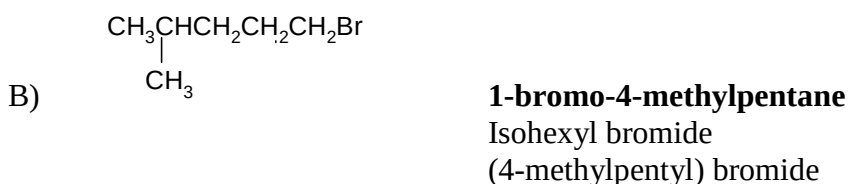
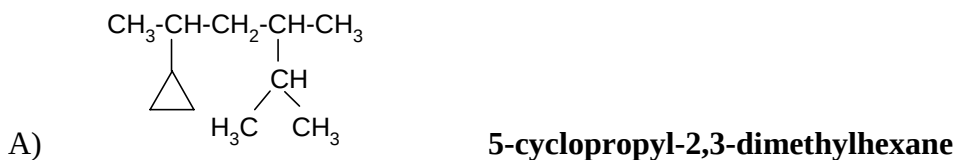
(Kahn, Summer 2002)

Midterm I:

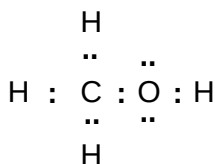
Answer Key

Section I. (50 points total)

1. Give a systematic name (4 points each; 20 pts total)



2. Draw Lewis (electron dot) structure for methanol. Determine formal charge for each atom. (5 pts)



$$Q(\text{H}) = 1 - (0 + 0.5 \cdot 2) = 0;$$

$$Q(\text{C}) = 4 - (0 + 0.5 \cdot 8) = 0;$$

$$Q(\text{O}) = 6 - (4 + 0.5 \cdot 4) = 0;$$

Every atom has formal charge of zero,

3. What atomic orbitals overlap to form the CH bonds in cyclopentane? (4 points)

sp^3 hybridized atomic orbital of carbon overlaps with the s atomic orbital of hydrogen

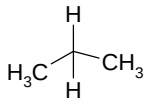
4. Rank the following molecules in the order of increasing dipole moments and briefly explain your reasoning (5 points).

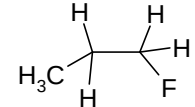
- A) 2-bromopropane
- B) Ethane
- C) 1-fluoropropane
- D) Propane

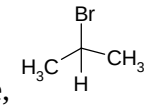
B < D < C < A

(3 pts for order, 2 pts for explanation)

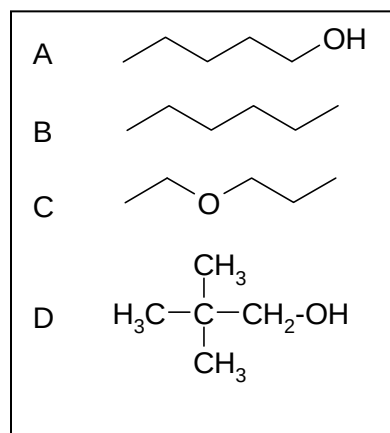
Ethane (in staggered conformation) has a center of symmetry and all small C-H dipoles cancel perfectly. $\mu = 0.00$ Debye

Propane, , does not have a center of symmetry and thus has a small dipole moment due to weakly polar C-H bonds. $\mu = 0.084$ Debye

1-Fluoropropane, , has a very polar C-F bond because fluorine is more electronegative than hydrogen or bromine. However, the C-F bond is shorter (1.40 Å) than the C-Br bond (1.93 Å) and the dipole moment ($\mu = \text{charge} \times \text{distance}$) of C-F bond is slightly smaller than that of C-Br bond. The experimental dipole moment of 1-fluoropropane is 1.95–2.05 Debye depending on the conformation. (*I know, this was a tough one*)

2-Bromopropane, , has the strongest dipole moment because the C-Br bond is both long and polar. $\mu = 2.20$ Debye.

5. Rank the following compounds in the order of solubilities in water. Briefly explain. (5 points) (3 pts for order, 2 pts for explanation)



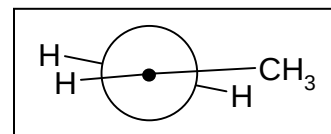
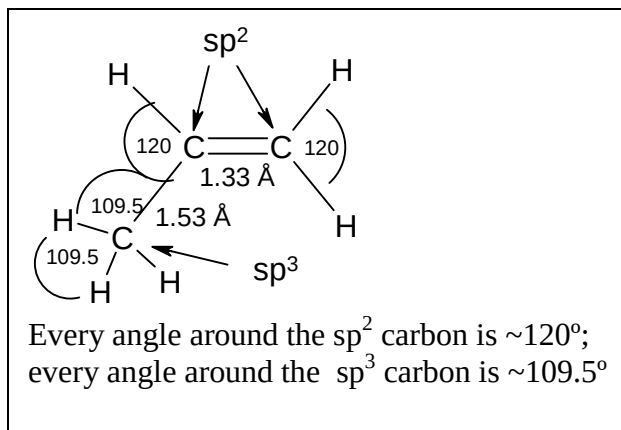
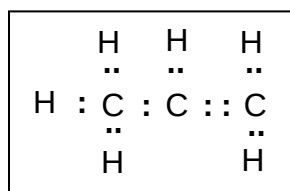
Most soluble **D > A > C > B** Least soluble

Branched alcohols are more soluble than linear alcohols. 2,2-dimethyl-1-propanol has infinite solubility in water while only 2.3–2.7 g of 1-pentanol can be dissolved in 100 g of water.

For the same number of carbons, alcohols tend to be more soluble than ethers in water because hydroxyl hydrogen can make good hydrogen bonds with water. Ethyl propyl ether has solubility of 1 (or 1.8, depending who you believe) g/100 g water.

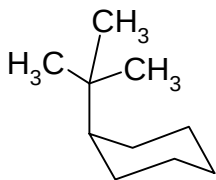
Alkanes are essentially insoluble in water. About 1 mg of hexane dissolves in 100 g of water.

6. Consider the structure of propene (8 points)
- Draw the Lewis (electron dot) and Kekule (bonds as lines) structures for propene
 - Indicate hybridization at each carbon atom
 - Show approximate distance values for every carbon–carbon bond
 - Show approximate values for every angle in this molecule
 - Draw the Newman projection of propene looking along the carbon–carbon double bond

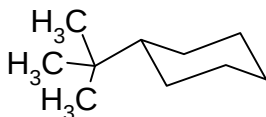


Four atoms H,H,H,C, connected to two sp^2 carbons are all in one plane.

7. Which of the two conformers is more stable. Why? (3 points)

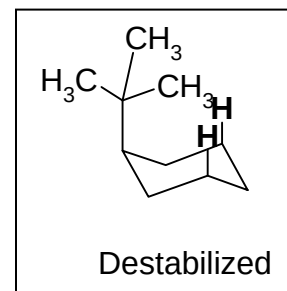


A



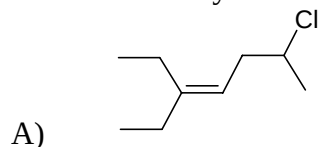
B

B is more stable
because conformer A is destabilized by 1,3-diaxial interactions with hydrogens as shown on the right:→
(Large) substituents prefer equatorial positions in substituted cyclohexane.

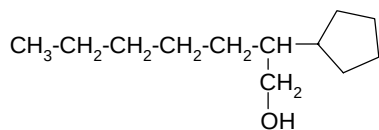


Section II. (30 points total)

8. Give a systematic name (5 points each)



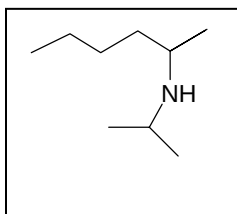
6-chloro-3-ethyl-3-heptene



B)

2-cyclopentyl-1-heptanol (must specify "1-")

C)



N-isopropyl-2-hexanamine

N-isopropyl-2-hexylamine

N-isopropyl-1-methylpentylamine

(but not "hexamine")

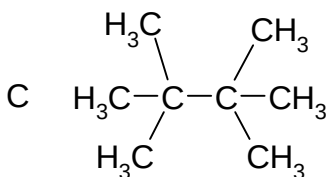
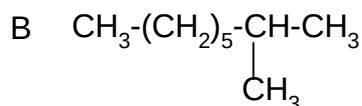
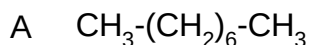
9. Write electronic configurations for carbon in the ground state and after promotion (in an excited state) (6 points)

Ground state: $1s^2 2s^2 2p^2$ **After promotion:** $1s^2 2s^1 2p^3$

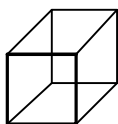
Note that promotion is not the same as hybridization. The electronic configuration after hybridization depends on what kind of hybridization occurred.

Arrow diagrams OK as long as they are correct. Must show also $1s^2$.

10. Predict order of melting points for the following four compounds and explain your reasoning. (9 points)



D



First, notice that the question is about **melting points**. Melting points are mainly determined by the efficiency of packing of molecules. The strength of intermolecular forces is also important.

High melting **D > C > A > B** Low melting

Cubane (D) molecules can be packed very tightly due to the regular shape of the molecule. It has the highest melting point (131 °C)

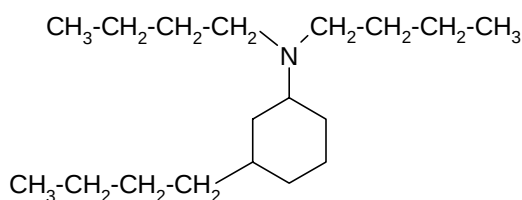
2,2,3,3-tetramethylbutane (C) has also fairly regular shape that allows efficient packing. It is solid at room temperature and melts in the boiling water (100 °C)

Octane (A) is a rod-like, but because the molecule is fairly flexible, the ideal packing is not easily achieved. It is liquid at room temperature and solidifies at −57 °C.

Isononane (B) has one more carbon than others but more importantly it is a branched molecule. Branching interferes with packing significantly and isononane is liquid that solidifies at −80 °C.

Section III. (20 points total)

11. Give a systematic name (4 pts)



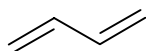
N,N,3-tributylcyclohexanamine

N,N,3-tributylcyclohexylamine (but not “hexamine”)

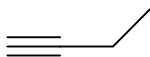
(N,N-dibutyl-3-butylcyclohexanamine gets 3.5 points)

(Do not need to specify position 1 as it is implied to have functional group.)

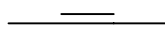
12. Draw structural formulas for all the possible isomers with empirical formula C_4H_6 . Name as many as you can. (8 pts)



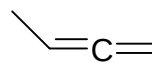
1,3-butadiene



1-butyne



2-butyne



1,2-butadiene



methylene-
cyclopropane



3-methyl-
cyclopropene



1-methyl-
cyclopropene

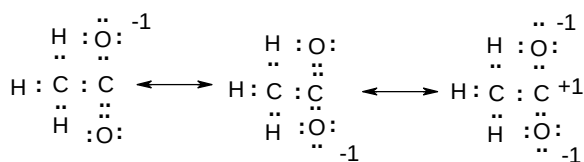


cyclobutene



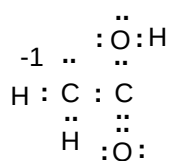
bicyclo[1.1.0]
butane

13. Draw Lewis (electron dot) structures for possible isomers for a **negatively charged ion** that has an empirical formula $C_2O_2H_3$ (8 pts)

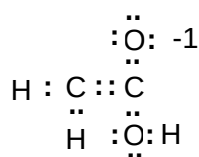


1) This is the acetate anion. The acetate anion has two equal resonance forms with formal negative charge on an oxygen atom. (3 or 4 points)

Each subsequent structure is 1 point:

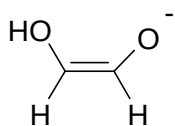
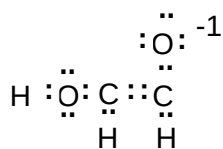


1a) This would be an unstable tautomer of acetate. Such a structure is unstable because here the negative charge resides in a less electronegative atom (C) instead of oxygen.

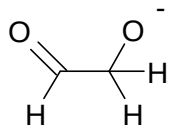
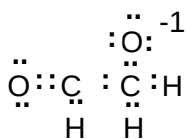


1b) This is a resonance structure for the tautomer shown in 1a. This resonance form is more stable than 1a because now the negative charge is at the oxygen atom.

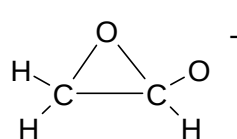
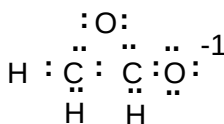
2, 3, 4, and 5.



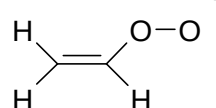
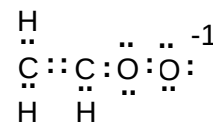
Anion of
1,2-ethenediol



Anion of
2-hydroxyethanal



Anion of oxiranol
(hydroxyoxirane)



Anion of
ethenyl hydroperoxide

6 and more: There are few more structures where the negative charge is at the carbon atom.

NOTE: The names were not required. They are given just for your information.