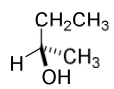
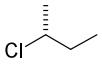
CHM 1321

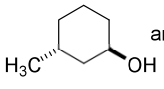
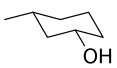
Mid Term 1 (February 4, 2011) Answers

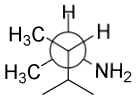
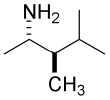
1) Identify the stereochemical relationship between the following molecules (enantiomers, diastereomers, same molecule, meso compound) (**4 Points**)

a)  and  relationship Same (1)

b)  and (S)-2-chlorobutane

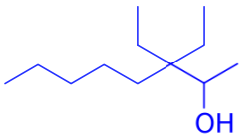
relationship Enantiomers (1)

c)  and  relationship Diastereomers (1)

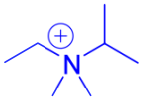
d)  and  relationship Diastereomers (1)

2) Draw the following as line structures: (**4 points**)

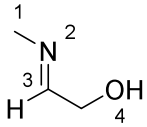
a) 3,3-diethyloctan-2-ol

 (2)

b) $[CH_3CH_2N(CH_3)_2CH(CH_3)_2]^+$

 (2)

3) For the following compound:



a) What is the hybridization of both carbons, the oxygen and of the nitrogen? (**4 points**)

C_1 = sp^3
N_2 = sp^2
C_3 = sp^2
O_4 = sp^3

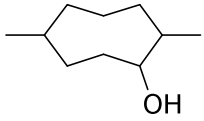
b) What is the geometry of both carbons, the oxygen and of the nitrogen? (**4 points**)

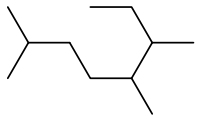
C_1 = tetrahedral
N_2 = trigonal
C_3 = trigonal
O_4 = tetrahedral

c) What molecular orbitals connect the following pairs of atoms? (**4 points**)

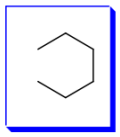
C_1 and N_2 = σ
N_2 and C_3 = $\sigma + \pi$
O_4 and H = σ

4) Give IUPAC names for the following: (**6 points**)

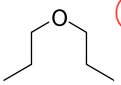
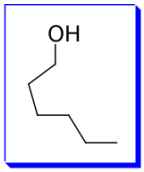
a)  2,6-dimethylcyclooctanol (3)

b)  2,5,6-trimethyloctane (3)

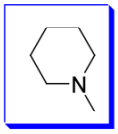
5) For each of the following pairs, circle the compound that best fits the criteria. Briefly justify your choice in each case. (**9 points**)

a)  (1) and  Which has the lowest boiling point? (2)

Both structures are capable of van der Waals interactions only.
First structure is an open-chain compound, second structure is a ring. Rings pack together better making crystal formation easier and melting more difficult.

b)  (1) and  Which is most soluble in water?

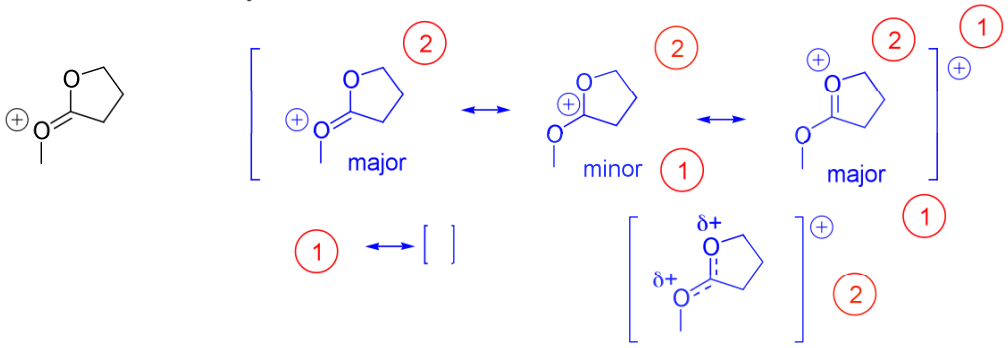
Second structure can hydrogen bond with water, and can participate fully (has hydrogen and lone pair)
First structure capable of hydrogen bonding with water, but only using lone pairs. The hydrogen bonding will be weaker for this compound.
The Second compound is capable of stronger hydrogen bonds with water, and so will be more soluble in water. (2)

c)  (1) and  Which has the highest boiling point?

(2)

Both structures are capable of van der Waals interactions
Second structure has a dipole and is capable of dipole-dipole interactions. These are stronger than VdW and so the second structure will have stronger intermolecular forces and a higher boiling point

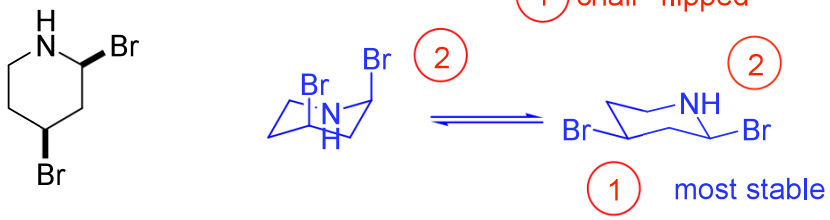
6) Draw the important resonance forms for the following. Identify the major and minor forms and show the resonance hybrid structure. (**12 points**)



(2) (2) (2) (1)
(1) (1) (2)

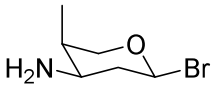
7) For the following:

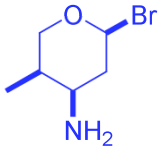
a) Draw <u>both</u> chair conformations of the following compound. Indicate which form is the most stable (**6 points**)



(1) chair "flipped" (2) (2) (1) most stable

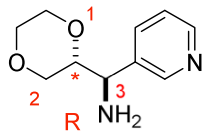
b) Draw the "flat" line structure of the following (be sure to indicate stereochemistry). (**3 points**)

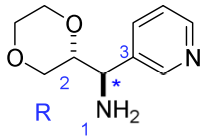




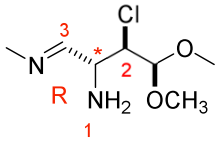
8) For the following compounds
   a) show the stereogenic centre(s) by labeling them with a star (*)(**4 points**)
   b) determine the priorities of the substituents on each stereogenic centre. For compounds with more than one centre, make sure you clearly indicate which priorities refer to which centre. (re-drawing the structure helps) (**8 points**)
   c) Determine the configuration of each stereocentre (**4 points**)

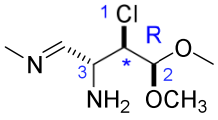
(i)





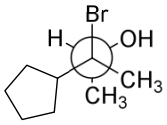
(ii)

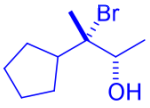




9) For each compound shown below, convert the structure to a zig-zag (line) notation. (**4 points**)

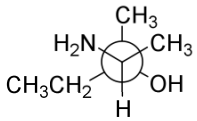
(a)

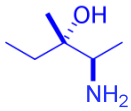




(2)

(b)





(2)

10) The specific rotation of the (R) form of Viagra is +40.0°. A third world drug maker is selling Viagra on the internet. To save money, the company makes a mixture of the active (R) form and the inactive (and toxic) (S) form. The FDA confiscates the shipment of this "counterfit" Viagra and measures the optical rotation. If the value of the specific rotation is -32°, what is the composition of the mixture (what % is the R form and what % is the S form)? (**7 points**)

the rotation of the sample will be negative so the S isomer is in excess

(1) optical purity = $\frac{[\alpha]_{sample}}{[\alpha]_{pure}}$ X 100 %

(1) 80 % = $\frac{32°}{40°}$ X 100 % (1)

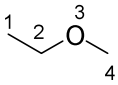
ee = optical purity = $\frac{|S - R|}{S + R}$ X 100 % (1) S + R = 100 (1)

(1) 80 % = $\frac{100 - 2R}{100}$ X 100 %

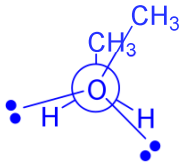
R = 10

Mixture is 10 % R isomer and 90 % S isomer (1)

11) For the following compound, draw the appropriate Newman projection along the O_3-C_2 bond of the following:



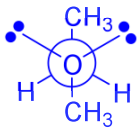
a) The least stable conformer and name the conformer. **(4 Points)**



3

Eclipsed (1)

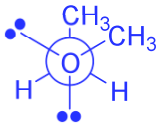
b) The most stable conformer and name the conformer. **(4 Points)**



3

Anti-Staggered (1)

c) The second most stable conformer and name the conformer. **(4 Points)**



3

Gauche Staggered (1)

Bonus: Which of the following is the weakest acid? You must justify your answer to get the marks. **(2 Points)**