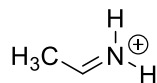
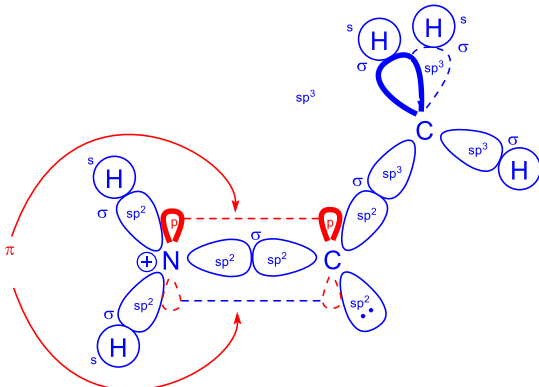


CHM 1321 A Mid Term 1 Version B Answers

1) For the following compound



a) Use the LCAO method to show orbital structure the compound (**6 Points**).



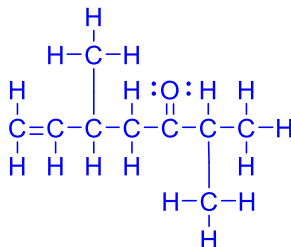
b) Label all the atomic orbitals used and the bonds formed in part a (**6 Points**).

2) Draw 2,5-dimethylhept-6-en-3-one as: (**6 points**)

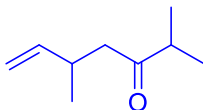
a) A condensed formula



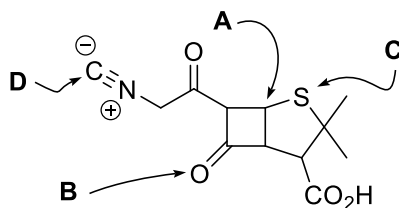
b) A Lewis structure



c) A line structure



3) For the following compound:



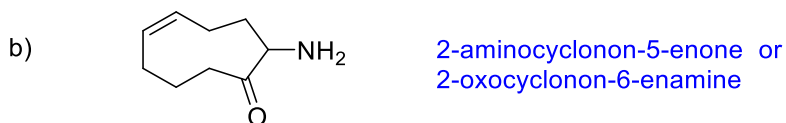
a) What is the hybridization of the indicated atoms? (**4 points**)

Atom A = sp^3
 Atom B = sp^2
 Atom C = sp^3
 Atom D = sp

b) What type of molecular orbitals connect the following atoms to other atoms? (6 points)

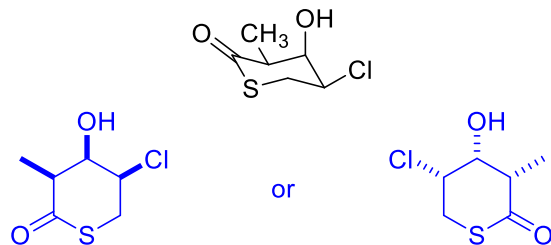
Atom A = σ
 Atom B = $\sigma + \pi$
 Atom C = σ
 Atom D = $\sigma + \pi$

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

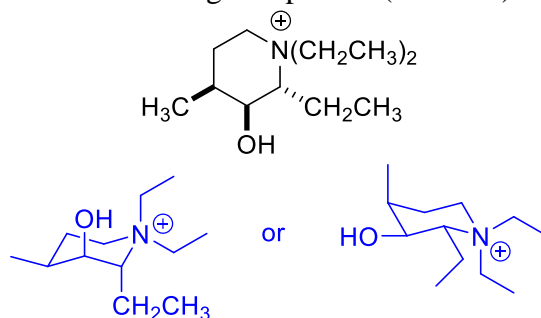


5) For the following:

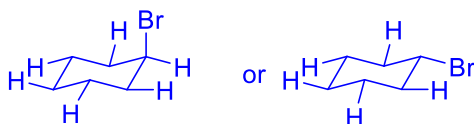
a) Draw the “hexagon” line structure of the following (be sure to indicate stereochemistry). (3 points)



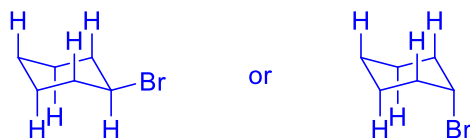
b) Draw one chair conformation of the following compound. (4 Points)



c) Draw one chair conformation of bromocyclohexane showing ALL OF THE EQUATORIAL HYDROGENS. (3 Points)



- d) Draw the other chair conformation of bromocyclohexane showing ALL OF THE AXIAL HYDROGENS. (3 Points)

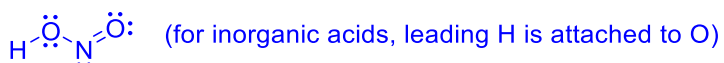
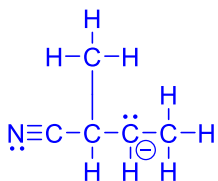
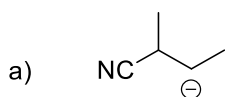


- e) Which of the two structures has the lowest energy and why? (2 Points)

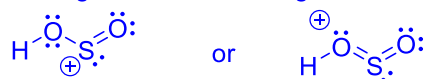
The lowest energy structure will be the one in which the Br is equatorial. Whether this is c or d depends on which chair you drew first.

The conformer in which the large group (Br) is in an equatorial position is most stable (lowest energy).

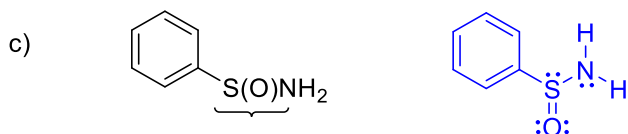
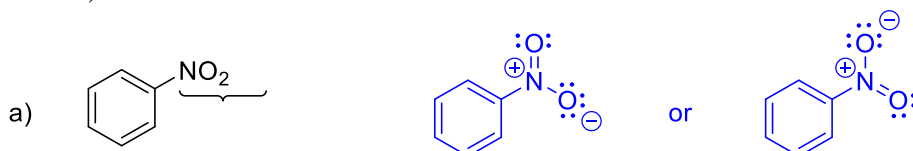
- 6) Draw the following molecules as Lewis structures. (6 points)



(for inorganic acids, leading H is attached to O)



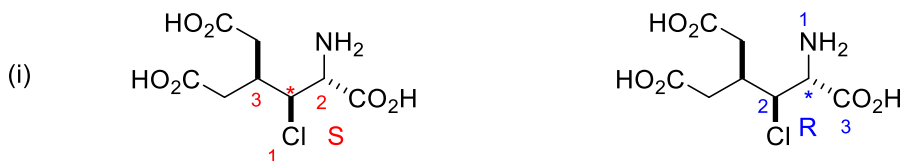
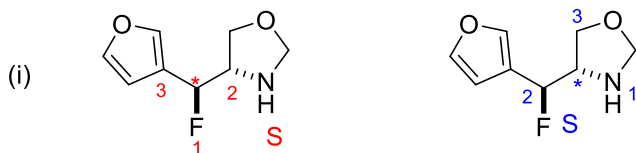
- 7) Re-draw the following molecules showing the full Lewis structure at the indicated location. (6 Points)



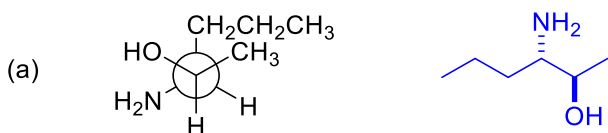
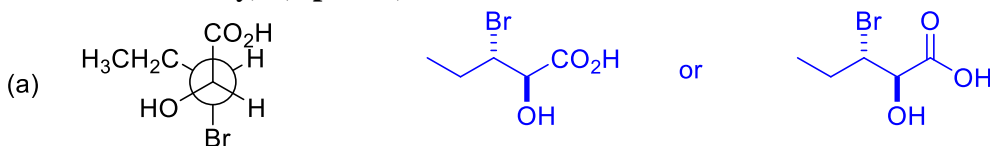
- 8) For the following compounds

- 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)**



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



- 10) A solution of 20.0 mg of (l)-glucose was dissolved in 5 mL of water and placed in a 100 mm cell. Using the sodium D line, a rotation of -0.031° was found at 22°C .

- a) What is the sample concentration in the units most commonly used for this measurement? **(3 Points)**

$$c = \frac{20.0 \text{ mg}}{5 \text{ mL}} \times \frac{\text{g}}{1000 \text{ mg}} \times \frac{100 \text{ mL}}{(100 \text{ mL})}$$

$$= 0.40 \text{ g/100 mL}$$

c is in units of g/100 mL (or g/dL)

- b) Determine the specific rotation of the sample. **(4 Points)**

$$[\alpha]_D^{22} = \frac{100 \alpha}{c \cdot l}$$

$$= \frac{(100)(-0.031)}{(1)(0.40)}$$

$$= -7.8^\circ$$

- 11) The specific rotation of the pure (R) form of Digoxin is -42.0° .

- a) What is the specific rotation of a 3 g sample that contains the (S) isomer of Digoxin in 96 % enantiomeric excess? **(3 points)**

$$ee = \text{optical purity} = \frac{[\alpha]_{\text{sample}}}{[\alpha]_{\text{pure}}} \times 100\%$$

$$96\% = \frac{[\alpha]_{\text{sample}}}{42} \times 100\%$$

$$[\alpha]_{\text{sample}} = +40.3^\circ \quad (\text{S isomer gives + rotation})$$

- b) What is the composition of the mixture (how much R form and how much S form)? (3 points)

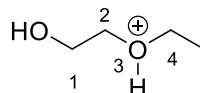
$$ee = \text{optical purity} = \frac{|d - l|}{d + l} \times 100\% \quad d + l = 100$$

$$96\% = \frac{|100 - 2l|}{100} \times 100\%$$

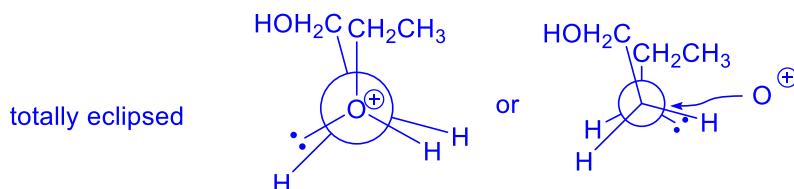
$$l = 2$$

Mixture is 98 % S isomer and 2 % R isomer

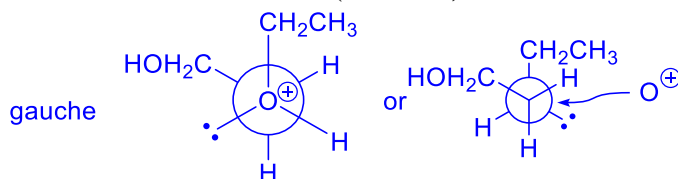
- 12) For the following compound, draw the appropriate Newman projection along the C2-O3 bond of the following:



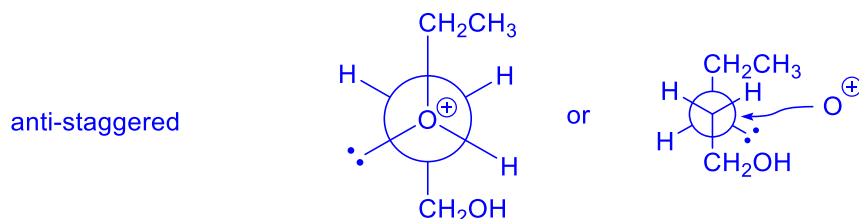
- a) The least stable conformer and name the conformer. (4 Points)



- b) The conformer that results after the structure in part a undergoes a 60° rotation about the C2-O3 bond and name the conformer. (4 Points)



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



BONUS! Draw the Newman projection of the following molecule as viewed along the C=O bond (it may be helpful to construct a model). (2 Points)

