

ANSWERS TO THE PRACTICE QUIZ, CHM222, SECTION I.

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1.1. The bromine atom is on carbon-1 and then an ethyl group is on carbon-2. The most stable form has these "big" groups anti to each other as shown in the Figure 1.

1.2. The least stable form with a local energy minimum is the gauche form, but the form in which the bromine atom is eclipsed with the ethyl group is the highest point on the potential energy curve – see Figure 1.

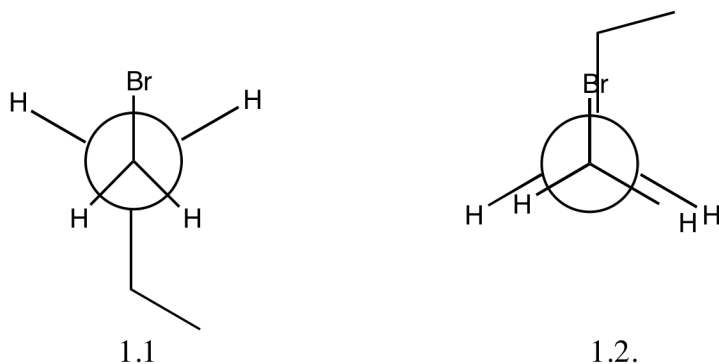


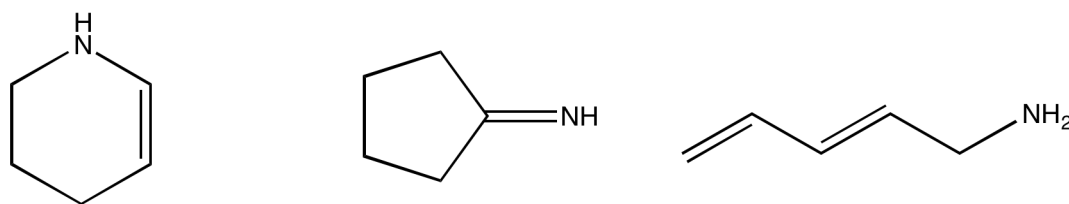
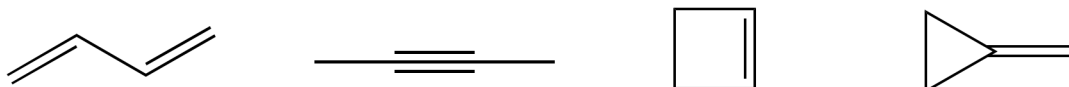
FIGURE 1. Newman structures for question 1.

2.1. The ihd is computed by taking the number of carbon atoms, doubling it, adding two, subtracting the actual number of hydrogen atoms, and finally dividing the previous result by two. If the molecule has a halogen, it is treated as if it were a H; if it has an oxygen, sulfur, etc., that is ignored. The only hard case is for N, P, etc. Then one of the H has to be taken out of the calculation. So, in this case $2 \cdot 5 + 2 = 12$; $12 - 8$ (taking away one of the H) = 4; divided by two yields an ihd of 4. There are two double bonds, or one double bond and one ring, or two rings in the compound.

2.2. Three possible structures are given in Figure 2.

2.3. This compound has an ihd of 2 also. So ring and double bond or two rings or two double bonds. See Figure 3.

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FIGURE 2. Three (of many) possible structures for C_5H_9N FIGURE 3. Four possible structures for C_4H_6

2.4. I would first compute the ihd to see what has to go into my structure. $(2 \cdot 4 \text{ C} + 2 - 2\text{H} - 4 \text{ Cl})/2 = 2$. So I need two double bonds without a C-C π bond – impossible, or a ring and a C=O. See Figure 4a.

3.1. An alcohol has an -OH group. See Figure 4b.

3.2. A ketone has a C=O. See Figure 4c.

3.3. An amine has an -NH₂ group. See Figure 4d.

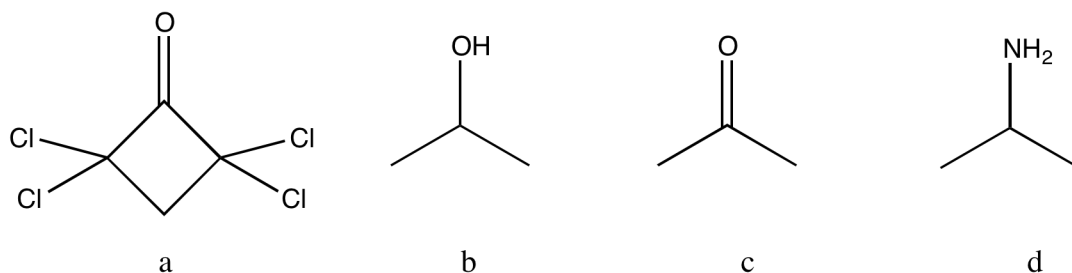


FIGURE 4. Answers to 2.4, and 3.

4. Numbering from the carbonyl carbon (because that is the correct thing to do), the carbon levels are 2, 0, 2, 1 because the first carbon has two bonds to an electronegative compound (O), the second none, the third 2 (to two F) and the last one. See Figure 5.

5.1. The carbon in methanal or thiomethanal is bonded to three other atoms; therefore sp^2 hybridization.

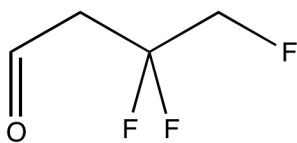


FIGURE 5. The compound of problem 4.

5.2. The most tightly held electrons are σ bonding electrons, followed by π bonding electrons, followed by lone pairs. Therefore, the HOMO of thiomethanal is a lone pair on the S. See Figure 6.

5.3. The LUMO must be an empty orbital that is relatively stable. Strong σ bonds give very unstable antibonds whereas weak π bonds give relatively stable empty antibonds. Therefore the LUMO is the π^* bond, localized more on C than on S. See Figure 6.

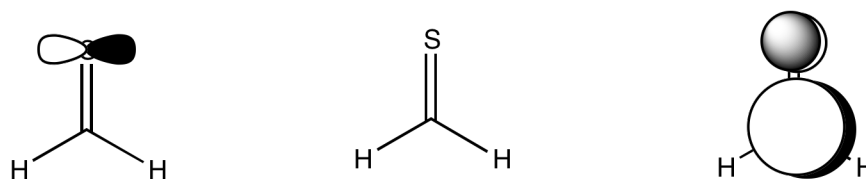


FIGURE 6. The homo, left, and lumo, right, of thiomethanal, Problem 5.

6. The carbon atom attached to the nitrogen is positive and is subject to attack by the negative charge on the hydride ion. The result is a shifting of negative charge to nitrogen. After this initial step, the negatively charged nitrogen atom is protonated.

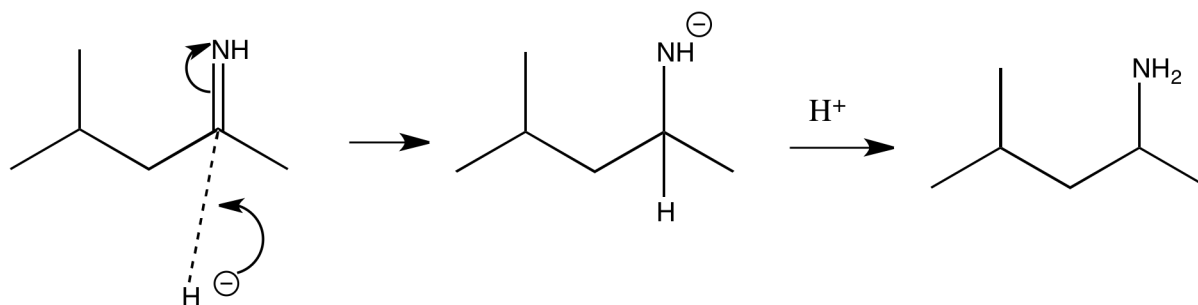


FIGURE 7. Mechanism for problem 6.

7.1. The peaks at 3050 cm^{-1} and 1610 cm^{-1} suggest a double bond with a $=\text{C-H}$ bond. The 1730 cm^{-1} suggests a carbonyl and the presence of the 2720 cm^{-1} indicates that the carbonyl may be an aldehyde.

7.2. The strong, broad $3000\text{-}3400\text{ cm}^{-1}$ suggests an -OH (or perhaps an NH) and the weak 2230 cm^{-1} indicates a C-C triple bond may be present.

7.3. The two broad peaks above 3000 cm^{-1} suggests an -NH_2 and the 1720 cm^{-1} a carbonyl. Together, they suggest an amide.

7.4. Nothing I want to suggest.