1. Using the spectroscopic reference information that is available in “SAM” as well as in Chapter 15 of the Jones text, propose an organic structure that is consistent with the spectral data shown below. Be sure to discuss as a group the major pieces of information and how the information is used to derive the structure.
2. Using the tables on pages 18-22 of “SAM” and the table inside the back cover of Jones, report an estimated pKa value for each hydrogen atom shown in each structure. Circle the most acidic hydrogen on each molecule.
3. Often times, amines are converted to their acid salts in order that they can be stored for long periods of time without degrading. One such example is shown below in which mescaline exists as a hydrochloride salt. Consider the reaction shown below between the protonated form of mescaline and NaOH.

\[
\begin{array}{c}
\text{MeO} \\
\text{OMe}
\end{array}
\text{H} \\
\text{Cl} \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \ quad
\end{array}
\text{NaOH}
\]  

Using the pair problem solving method (as explained by your workshop leader), answer the following directives. Note: each directive has been labeled with an A or B to indicate the task of each person in the pair.

**A:** Show all hydrogen atoms in protonated mescaline and report the pKa values (from the tables in “SAM” or from the inside back cover of Jones). Circle the most acidic hydrogen and explain your choice.

**B:** Realizing that NaOH dissociates into ions, draw the Lewis structure for hydroxide anion.

**A:** The hydroxide anion exists as a major reactive species in solution and functions as the Bronsted-Lowry base in the forward direction. Use the curved-arrow formalism to show the flow of electrons as the reaction proceeds from reactants to products (forward direction).

**A:** Draw the structures for the expected products of this reaction based upon the mechanism you derived.

**B:** Which species is your nucleophile (Lewis base) and which is your electrophile (Lewis acid) in the forward direction? Which species will donate electrons via its HOMO and which will use its LUMO to accept the electron pair? Briefly explain your choices.

**A:** Report the appropriate pK_a value to use for the “other acid” (on the product side of the of your equilibrium reaction).

**B:** Designate each of the species in your reaction as a strong acid (SA), strong base (SB), weak acid (WA), or weak base (WB). Explain your rationale.

**B:** Show the conjugate acid-base pairs.

**A:** Calculate the overall pK_a (from the individual pK_a’s) and convert to the K_a.

\[
pK_a (\text{overall}) = pK_a (\text{forward rxn}) - pK_a (\text{reverse rxn})
\]

**B:** Use the K_a from the previous answer to find \( \Delta G°_{rxn} \) at room temperature (23 °C).

**B:** Which species (products or reactants) are favored at equilibrium? Explain.