Full Interpretation of IR and NMR Spectra

^{13}C NMR Interpretation

1. Compute the unsaturation number or rings (SODAR) from the composition of the molecule in order to gain an appreciation of the complexity of the unsaturation or rings in the molecule. Note the information concerning the chemical composition of the structure being analyzed. If the composition is given, compute the "number of unsaturated units or rings" from the composition $C_xH_yN_z$:

   $UR = (x + 1) - y/2 + z/2$

   In this formula, halogens are equivalent to hydrogens. Oxygen atoms do not enter into the calculation.

   Examples: (1) C_6H_{14}: $UR = (6 + 1) - 14/2 = 7 - 7 = 0$. This is a saturated hydrocarbon.

   (2) C_6H_{12}: $UR = (6 + 1) - 12/2 = 7 - 6 = 1$. The structure contains a single ring or a C=C bond.

   (3) C_6H_6: $UR = (6 + 1) - 6/2 = 7 - 3 = 4$. The structure contains some combination of rings and/or double bonds and or triple bonds that add up to 4 units. For example, benzene possesses one ring and three double bonds (4 units) and is an acceptable structure. A SODAR of 4 is characteristic of a benzene ring.

2. Note the general groupings of signals and assume that signals which possess similar chemical shifts correspond to similar carbon atoms in the moleclue.

3. **Count the number of distinct peaks in the spectrum.** This is equal to the minimum number of chemically different carbon atoms in the molecule, N_c. The more peaks, the higher the complexity. There may be more carbon atoms than this number only if two carbon atoms happen, by accident, to have the same chemical shift.

3. **Assign each of the carbon atoms to a functional group type based on information from a standard table of chemical shifts.** Remember that the values in the Table are approximate and an exact match is unlikely. However, from experience you will become accustomed to the maximum deviation which signals a poor correlation.

4. The areas under the peaks in ^{13}C NMR **do not** correspond to the actual number of carbon atoms in the molecule (although the opposite is true for ^{1}H NMR). In general, however, there is a clue to the kinds of hydrogens attached to a carbon atom that can be taken from the size of the peaks. If there is one or more hydrogens directly attached to the carbon atom, the

size of the peak tends to be strong. If there are no hydrogens attached to the carbon atom, the size of the peak tends to be weak.

5. Try to piece together a structure which is consistent with the number of peaks, their chemical shifts and the relative sizes of the peaks.

6. Go to the IR and ^{1}H NMR for confirmation.

7. A detailed IR analysis has been discussed in Handout 18.

^{1}H NMR Interpretation

8. Note the general groupings of signals and assume that peaks which possess similar chemical shifts correspond to similar protons atoms in the moleclue or to the multiplet spin-spin splitting pattern of an equivalent group of protons. Sharp singlets with rare exceptions correspond to structurally equivalent protons.

9. Use the areas under the various absorptions to estimate the number of similar protons of each type.

10. Use all of the information to postulate plausible test structures. A plausible test molecular structure must be consistent with the moleular formula, the UR number, the carbon number N_c, and the chemical shifts. In addition, the test structure must be consistent with information in the IR spectrum.

11. Challenge each of the test structures with the predictions of the multiplets which are approximate first order splittings.