Possible approach for solving a structure problem:

IF YOU HAVE ACCESS TO 1D NMR DATA, AN IR SPECTRUM AND A MOLECULAR WEIGHT

1. Try to get a molecular formula and calculate the degrees of unsaturation.
   a. In a typical problem you will be given a H and C/DEPT NMR, an IR and a MS or a MW.
   b. Count the number of protons from the H NMR spectra. Integration shows ALL protons present.
   c. Count the number of carbons from the C NMR spectra. Can you spot any symmetry? This is important because in decoupled C NMR we only see each type of carbon and integration can be unreliable.
   d. If no mass spec (MS) is given, then you will be given the molecular weight and the number of halogens and/or sulfur atoms. An odd MW means there is an odd number of nitrogen atoms (1, 3, 5, etc).
   e. Subtract the C,H and halogen/sulfur mass from the molecular weight (given from MS) and estimate the number of N and O present (use exact masses: N=14, O=16, S = 32, Cl = 35, Br = 79, I = 127). Look for clues for these atoms in the other spectra. The IR and C-NMR are very helpful at identifying functional groups that are present. Some groups are easier to see in the IR (nitrile and nitro are a couple).
   f. Once you have a molecular formula, calculate the degrees of unsaturation (pi bonds and/or rings).
2. Estimate the number of pi bonds from the C NMR (C=C, C=O, N=O, nitrile, alkyne, aromatic, etc.) and subtract the number of pi bonds from the total degree of unsaturation. The difference should be the number of rings in the structure. Look for supporting evidence in the IR, H and C NMR. If you have alkene and/or aromatic pi bonds, use the sp^2 CH bend region (600-1000 cm^{-1}) to see if you can identify substitution patterns of the pi systems. Check H NMR chemical shifts and coupling constants for consistency.
3. Tabulate and identify each carbon type using the DEPT. Recheck the number of protons and carbon atoms using the DEPT. Any protons on oxygen or nitrogen will not show up in the DEPT and this may provide clues about the number of O-H and N-H bonds. Look for supporting evidence in the IR and H-NMR spectra.
4. Carefully analyze the H NMR chemical shifts and multiplicities. Try to reduce pieces of the puzzle, looking for overlapping parts using multiplicities and coupling constants (J values) to join individual pieces together. Look for shielding and deshielding effects on protons and carbons.

IF YOU HAVE ACCESS TO 2D NMR DATA

5. Use the COSY to generate paths of connectivity among the protons (also called “spin systems”).
6. Use the HETCOR or HSQC to identify which protons are on which carbons. These experiments look at one bond coupling (^1J) between carbon and hydrogen and pairs the H from the COSY with their carbons.
7. Use the HMBC (looks at 2 and 3 bond C-H coupling, ^2J, ^3J) to connect the COSY spin systems through any quaternary centers (carbons without any protons). Allows quaternary Cs to see their proton neighbors. And stitch together the various spin systems.
8. Double check your structure for consistency of chemical shifts and multiplicities in the H and C NMRs and functional groups showing in the IR.

Workpage for structure problems (on a separate page show work for ^{1}H NMR fragments, IR and formula)

^{13}C	DEPT structural unit	HETCOR	COSY	HMBC, NOE, other	^{1}H fragments from ^{1}H NMR