Experiment C: Introduction to IR & NMR Spectroscopy

Background
Spectroscopy is the most important tool in organic chemistry for distinguishing and identifying chemical compounds. The most important spectroscopic techniques in organic chemistry are $^1$H NMR and IR spectroscopy, closely followed by $^{13}$C NMR and mass spectrometry. Your instructor will provide background information and instruction as to how to interpret $^1$H NMR and IR spectra.

Reading
McMurry Chapter 12.5-12.8, 13 (or any other organic chemistry textbook chapters on IR and NMR spectroscopy).

Pavia 5th edition, Chapters 2, 5 and 7.

Chem 113A website, under Course Handouts - ‘Reporting NMR Spectral Data’ and ‘Reporting IR Spectral Data’.

Chem 113A Class Notes, pages B25-B62.

Prelab:
Experiment C is a "dry-lab" experiment, meaning no lab work is involved. There is no PreLab writeup nor an Experiment Summary Sheet for Experiment C. However, you are expected to include your data and analysis in your notebook (see below).

Procedure:

On the day of the "in-class exercise" for Exp. C, you will be provided with 2 sets of IR and NMR spectra; each set will correspond to a unique structure. You will also be provided with a list of the possible structures that will match each set of spectra given to the class. During the lab period, you will analyze your own spectral data and decide which of the structures match each of your 2 sets of data. I encourage you to work cooperatively with your classmates - everyone has a different set of data, so you can learn from observing data that is different from yours.

Experiment C is "open book" for your Pavia text only (no other source of information is allowed). You must have your own copy of Pavia. During the in-class exercise, all books, smartphones, computers/web-accessible devices, backpacks, etc, must be placed in the front of the room.

On your spectra, you should be assigning the peaks the correspond to your structures. At the end of the class period, show me your assignments (I may or may not indicate if they are correct).
IN YOUR NOTEBOOK:
Record your Unknown Codes.
Prepare Tables for both sets of IR and NMR spectra you obtain (see "Reporting IR Data" and "Reporting NMR Data" on the Chem 113A website, under the "Course Handouts" menu. When you have determined which structure matches your data, summarize your spectral assignments in your notebook. This will be the basis for a more detailed explanation in your Writeup (see below).

WRITEUP:
Experiment C involves only investigative aspects (no reaction or mechanism involved).

In your write-up, for each of the 2 compounds you are assigning, give an analysis and explanation of why your structure matches the IR and NMR data. Do not simply list the data and state that it "fits" for that compound - you must give an analysis of how each piece of data justifies a part of your structure. For example, for NMR explain how the chemical shift, integration and coupling pattern of a peak fits for a specific hydrogen (or set of hydrogens) in your structure; do this for ALL hydrogens in your structure. Similarly, explain as much of the IR data as possible. For IR, focus on the key peaks that support your structure (usually the peaks above 1400 cm\(^{-1}\), but in some cases peaks <1400 cm\(^{-1}\) may be useful.

At the end of the analysis in your writeup:

A. Summarize all of your IR and NMR data and assignments in tabular form using the format given in the Chem 113A website "Course Handouts" under "Reporting IR data" and "Reporting NMR data". You must follow these formats for IR and NMR data in your report.

AND

B. For all of your IR and NMR spectra, draw your structure on the spectrum and clearly indicate which peak corresponds to which part of your structure. Follow the format for IR spectra seen in Pavia: for NMR spectra a good example is seen on page B51 in the Chem 113A Class Notes. Label any solvent peaks or the TMS peak in the NMR. Turn in all your assigned spectra with your writeup.

Ideally, you will come up with one structure for each of your unknowns, but if there seems to be any ambiguity or difficulty with the spectral assignment, you may include footnotes explaining what the problem is, and how you attempted to resolve the issue.