SPECTROSCOPY

Note: No pre-laboratory summary or quiz is required for this laboratory activity, however you should review spectroscopy lecture notes and the related parts of the model activity. You should also review the "fragment approach" for solving spectroscopy problems. The laboratory period is more like a tutorial, "open book", you can work in groups(3 or 4) and ask your TA about any concepts you don't understand.

You should bring a calculator and a copy of the spectroscopy tables (see link below), model kit and you might also want to bring copies of your lecture notes.

The graded component of this F24 laboratory activity is on an online Moodle "spectroscopy worksheet" (50 min. time limit) that is to be completed by 18:30 MONDAY NOV 25th 2024.
Make sure you have stable internet when you start the graded activity and avoid the IT back-up hours (see information about the activity in Moodle)

OTHER DOCUMENTS:
Spectroscopy tables spectroscopy fragment approach spectroscopy worksheet, sample "exam" question

INTRODUCTION

This laboratory exercise provides an opportunity for you to get some practice with the problem solving skills associated with the elucidation of structure from spectral data and experimental data. **The exercise is designed to improve your understanding of how to tackle the identification of organic compounds based on their spectral characteristics. It maybe your first opportunity to learn how to do this effectively, including evaluating elemental analysis data.** Problem solving skills are very important in scientific research and development and for many other disciplines. In particular, spectroscopy is an important topic for chemistry but it also has applications in other sciences, medicine and engineering for example. Ch13 in the etext covers "Spectroscopy". There are also multiple self-assessment activities in Moodle on topics from Spectroscopy.

During the laboratory session, there will be an opportunity to review of index of hydrogen deficiency (IHD), counting types of H and C, and the use of combustion data and elemental analysis data. Each of these can be useful in the determination of structure from experimental and spectroscopic data.

Here is an example of a spectroscopy question of the type you will encounter on assessments (CAL assignment, Final examination). Note that we expect you to be able to solve these types of problems by the time the Final examination rolls around typically **in 20 minutes or less**. This will be after a few weeks of lectures on spectroscopy, this introductory laboratory exercise and the CAL practice and assignment. Also note that the spectroscopy tables provided for this experiment are also provided with examinations, so you don't need to memorise the tables.

GROUP ACTIVITY COMPONENT

You will be split up into small groups (ideally groups of 4) so that you can work on the spectroscopy worksheet. Remember that the aim is to help you to develop some of your spectroscopy problem solving skills and learn more about interpretation of spectra in order to deduce important and useful structural data.

As part of this you will also work on a spectroscopy problem (of the same format as CAL assignment 4 and Final examination written answer problem). The aim is to extract the important and useful structural data – with some guidance from your laboratory instructor – and work out the structure of the unknown compound. Your laboratory instructor will be there to answer your questions and help you develop your spectroscopic skill set as you work through the work sheet.

A METHOD FOR SOLVING SPECTRAL PROBLEMS

While there is no "specific" method that will work *every* time, there is a general approach, we call it the "fragment approach". The initial goal should be to determine the molecular formula whenever possible, then the component pieces, and finally a unique structure that is consistent with all the spectroscopic data. Remember that you don't need to use one information source on its own, other spectra should be able to provide supporting evidence, and remember that they have to be consistent: for example, if the molecular formula doesn't have oxygen, then there can not be a carbonyl group (*i.e.* C=O) in the IR! The more spectroscopy you know, the easier and less ambiguous the process becomes.

REFERENCES

1. For more practice spectroscopy problems see the materials contained in Chapter 13 of our Organic Chemistry etext: https://www.chem.ucalgary.ca/courses/351/Carey5th/Ch13/ch13-0.html
2. D.L. Pavia, G.M. Lampman, and G.S. Kriz, "Introduction of Spectroscopy", Saunders College Publishing, 1st ed. 1979, 2nd ed. 1996, 3rd ed. 2001.