

Infrared and Raman Spectroscopy for the Identification of Drugs

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Practical:

- Summary:**
1. Students carry out the exercise at Monash as part of a level 2 subject "Instrumental and Forensic Chemistry" although it appropriate for any subject that covers the theory and practical use of infrared and Raman spectroscopy. The notes are written in the context of Forensic science and this context appeals to most students. In this exercise students firstly reinforce their knowledge of vibrational spectroscopy theory using a computer program, record IR and Raman spectra of a common pharmaceutical drug and then identify the drug using a searchable database.

The aims of the practical are as follows:

- Using a computer simulation program Animol
1. Investigate the spectra of small molecules and correlate the bands with vibrational modes.
 2. Obtain a prediction of vibrational spectra of aspirin (acetyl salicylate), salicylic acid and paracetamol (4-hydroxyacetanilide) and compare the spectra. *Note. These could be any useful molecules you wish to enter into the Animol program.*

Record the infrared spectrum of a common pharmaceutical drug using a KBr matrix technique.

Search an infrared spectral database to identify the drug.

Record or obtain the Raman spectrum of a common pharmaceutical drug.

Search a Raman database to identify the drug.

Gain experience in data transfer and spectral manipulation.

The use of the computer simulation program allows the students to reinforce their theoretical knowledge whilst visualizing vibrational modes and relating these modes directly to predicted spectra. Students then have control over their rate of learning and depth of learning. The experimental part is straightforward and kept simple because it is often the first time students have used IR and Raman spectroscopy. The nature of the experiment can allow them to learn about the instrumentation, although this can be de-emphasized for students not involved in instrumentation. Although students should satisfactorily

identify the drug in question through database searching they will realise through the practical that a depth of knowledge is required to search the database and achieve the correct result.

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Discipline:Chemistry

Abstract

The experiment is closely linked to the “Instrumental and Forensic Chemistry” subject at Monash although it would be equally at home in any analytical spectroscopy, physical chemistry or analysis course. Even students doing courses in synthetic chemistry would find this a useful exercise.

Students require knowledge of the theory and instrumentation of IR and Raman spectroscopy and the ability to quickly come to terms with an interactive computer program. The sample preparation for the infrared requires a little skill that is picked up by most students quickly. They also require a familiarity with, or a desire to learn how to transfer data between computers and how to find their way around new computer packages.

Duration

Prior to Lab 30 min

In Laboratory 5 hours

After Laboratory 1 hour

Further comments

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