Experiment 1

Lab Safety & IR Spectroscopy


There is no prelab or lab report for today’s experiment. During today’s lab, you will check into a lab drawer. Your TA will then present information about lab safety and give you a safety quiz. Next, your TA will present a recitation on IR spectroscopy, an important technique used by chemists to help identify organic compounds. Finally, you will work on an in-class IR spectroscopy exercise (due at the next lab meeting). While you are working on the worksheet, your TA will take small groups to the IR instrument and demonstrate its proper operation, so that you can collect a spectrum of an unknown sample. Instructions for collecting an IR sample’s spectrum are given in the Handbook. For this experiment, and for everything you turn in during this course, you must do all the work on your own. You may discuss the assignment with your labmates, but everything you turn in must be exclusively your own work and nobody else’s.

While you are preparing for this experiment, or any other experiment in this course, you should make sure to read the recommend sections of the Handbook for Organic Chemistry that are listed just below the experiment’s title. These sections explain the background information and theory you will need to know in order to understand the material, and to earn a good grade on the lab report (if there is one for that experiment) and prelab quiz (if there is one for that experiment). The reading for this experiment includes material on lab safety and IR spectroscopy. You should also refer to the listed sections of your textbook - either Loudon or Clayden et al., depending on which textbook you are using.

Chemical Structures and Functional Groups

During this experiment, you will see molecules depicted in ways you might not be used to. These are called skeletal, line-bond or zigzag formulas. In this system, every bend or end of a line is a carbon unless explicitly stated otherwise. Hydrogen atoms are assumed to be present in the amount needed to fill octets, unless there’s a charge on the atom that implies it does not have a filled octet. All heteroatoms (atoms other than C and H) must be shown explicitly, but any C or H can be shown explicitly if necessary. However, if an atom is shown explicitly, its H atoms must also be shown (Figure 1-1).

![Figure 1-1: Some examples of skeletal structures.](image-url)
Note that we have a choice in how much to show explicitly, depending on what parts of the molecule we’re focusing on. In the last example here, the H that’s shown happens to be important for a particular reaction.

Functional groups (FGs) are small groups of atoms that react in a particular characteristic way, usually with no regard for what the rest of the molecule looks like. For example, all alcohols have an –OH group. The rest of the molecule is sometimes just abbreviated as R. (Figure 1-2)

![Figure 1-2: Some example of molecules with an alcohol functional group.](image1)

A subcategory of R is anything based on an aromatic ring. These are called aryl groups, or Ar for short (Figure 1-3). As far as we’re concerned for now, this is anything with a six-carbon ring of alternating double and single bonds. Aromatic double bonds can also be drawn as a circle.

![Figure 1-3: Some examples of molecules with aromatic rings.](image2)

The functional groups that you will see in the next few experiments are shown in Figure 1-4.

![Figure 1-4: Some functional groups you will see in this experiment and others.](image3)

These FGs have characteristic frequencies which show up in an IR spectrum. These are given in the table below, and you will be expected to know these for future labs.

### Key IR frequencies which you should memorize

<table>
<thead>
<tr>
<th>Frequency Range (cm⁻¹)</th>
<th>Functional Group/Example</th>
<th>Key IR Frequency Characteristics</th>
</tr>
</thead>
<tbody>
<tr>
<td>3400-3250 cm⁻¹</td>
<td>N-H – 1° and 2° amines</td>
<td>2830-2695 cm⁻¹ C-H aldehydes</td>
</tr>
<tr>
<td>3500-3200 cm⁻¹</td>
<td>O-H – alcohols, carboxylic acids</td>
<td>1750-1665 cm⁻¹ C=O – carbonyls (one sharp, narrow peak per carbonyl)</td>
</tr>
<tr>
<td>3100-3000 cm⁻¹</td>
<td>C-H – alkenes, aromatics</td>
<td>1600-1585 cm⁻¹ C-C – aromatics</td>
</tr>
<tr>
<td>3000-2850 cm⁻¹</td>
<td>C-H – alkanes</td>
<td>1500-1400 cm⁻¹ C-C – aromatics</td>
</tr>
<tr>
<td>2900-2850 cm⁻¹</td>
<td>C-H – alkanes</td>
<td></td>
</tr>
<tr>
<td>2800-2650 cm⁻¹</td>
<td>C-H – alkanes</td>
<td></td>
</tr>
<tr>
<td>2100-1600 cm⁻¹</td>
<td>C=C – alkynes, aromatics</td>
<td></td>
</tr>
<tr>
<td>1800-1500 cm⁻¹</td>
<td>C=C – alkynes, aromatics</td>
<td></td>
</tr>
<tr>
<td>1400-1200 cm⁻¹</td>
<td>C=C – alkynes, aromatics</td>
<td></td>
</tr>
<tr>
<td>1200-1000 cm⁻¹</td>
<td>C=C – alkynes, aromatics</td>
<td></td>
</tr>
<tr>
<td>1000-800 cm⁻¹</td>
<td>C=C – alkynes, aromatics</td>
<td></td>
</tr>
<tr>
<td>800-600 cm⁻¹</td>
<td>C=C – alkynes, aromatics</td>
<td></td>
</tr>
</tbody>
</table>
Name________________________________________

IR Exercise

Part 1
Your TA will assign you one of 8 unknown compounds, shown below. Collect an IR spectrum of your unknown and label its major diagnostic peaks; use this to identify your compound. Attach your spectrum to this worksheet. (5 pts for correct identity, 5 pts for labeling peaks)

Your unknown number: _____   What compound you think it is: __________________________

- 4-Heptanone
- Phenethyl alcohol
- Isopentyl acetate
- Morpholine
- N-Methylaniline
- 1-Octene
- Decane
- 1-Propanol

Part 2
Ten compounds and ten spectra are shown below. Match each compound with its IR spectrum and label the major diagnostic peaks in each spectrum to verify your assignment. (10 pts for correct identities, 10 pts for labeling peaks)

- Benzyl alcohol
- N-methylcyclohexylamine
- Aniline
- Acetophenone
- 3-Pentanone
- Ethyl acetate
- 1-Hexene
- 1-Butanol
- Pentane
- Butyraldehyde