Report Form
Exploring Infrared Spectroscopy

Part 1. Identifying an Unknown Compound.

The molecules whose spectra appear on pages 3 and 4 of the Experimental Directions are shown here. The objective is to match the molecule with its spectrum. For each spectrum identify the molecule and briefly describe your reasoning. That is, find bands in the spectrum that may correspond to the important functional groups. In your discussion identify a particular band (giving its wavelength in cm⁻¹ units) and specify the portion of the molecule giving rise to that band.

Spectrum A corresponds to _________________________________________ Explain briefly.

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Grade and Instructor Comments

Revised: March 2001
Spectrum B corresponds to ________________________________ Explain briefly.

Spectrum C corresponds to ________________________________ Explain briefly.

Spectrum D corresponds to ________________________________ Explain briefly.

Part 2. Spectra of CHCl₃ and CDCl₃

a) What are the positions of the C–H and C–D stretching bands?
   C–H = _________________ cm⁻¹    C–D = _________________ cm⁻¹

b) Explain why one of the stretching bands has a lower energy than the other. (Hint: think about the effect of the mass of the vibrating atoms on the energy of the vibration. See introductory materials.)
PART 3. Identifying a Packaging Film

Describe the prominent bands in the spectrum of your film and attempt to identify the film by matching it with the spectra of representative films.

Note: Attach the original spectrum to the report form of Team Member 1.

Part 4. Connecting IR Bands with Vibrations

a) Acetylene (filename = ACETYLEN.CSF)
   What is the structure of acetylene? (Make a sketch)

To what motion is the strong band at about 3400 cm\(^{-1}\) due?

Click on the little triangle at about 2200 cm\(^{-1}\). Why do you think this vibration (a symmetrical stretch along the axis of the molecule) does not give rise to an IR band?

To what motion is the strong band at about 1000 cm\(^{-1}\) due?

See the directions for using the CAChe models in the experimental directions handout. Note that these spectra can only be observed on the Macintosh computers. Please use one of the new iMacs in the lab.
b) Formaldehyde (filename = FORMALDE.CSF)
   Sketch the structure of formaldehyde.

   Into what class of organic compounds does this molecule fit? (See the summary table on page 6 of the introductory material.)

   Describe the vibration that gives rise to the strong band at about 2000 cm\(^{-1}\).

   Describe the vibration that gives rise to the weaker band at about 1000 cm\(^{-1}\).

   c) Based on your answers to the questions above regarding acetylene and formaldehyde, what can you conclude about the relative energies of bond stretching and bond bending vibrations?
Part 5. The Mystery Compound

You have decided you love Oneonta so much you are going to leave Long Island for good and move into a big old farmhouse near Oneonta. The place is cheap, though, because the natives tell you the owner was murdered in the house in 1918—but no one was ever caught nor do they know how he was killed. When you move in you find a bottle of evil smelling liquid hidden in the dark recesses of the damp basement. You decide you want to identify this liquid because, who knows, it might be the murder weapon! So, you bring your sample to the wonderful SUCO Chemistry Department where you know they can give you an answer. Your lab instructor first determines that the liquid is pure, and then runs an infrared spectrum. He tells you it is one of about 20 possible compounds.

a) Using the library of spectra available in the lab (and in a notebook in the Chemistry Computer Lab) decide on the identity of the compound. Explain your reasoning.

b) Go to internet and look up the MSDS sheet (Materials Safety Data Sheet) for your unknown compound. There are a number of places where these can be found. Among them are:

- http://siri.uvm.edu/msds/
- http://msds.pdc.cornell.edu/msdssrch.asp
- http://research.nwsc.noaa.gov/msds.html
- http://www.msdsonline.com

MSDS sheets are forms put out by manufacturers of pure chemicals (e.g., HCl, acetone) and chemical-containing products (e.g., WD-40). Listed are their physical properties, fire and explosion hazards, health hazards, and what to do in the event of a spill of the chemical.

Once there, type the name of your compound in the search box. Is your unknown compound listed as a hazardous material? Could it have been the murder “weapon?” (List some of the hazards and symptoms of overexposure.)