Infrared Spectroscopy

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Infrared spectroscopy is an instrumental method of analysis that can be used to identify and quantify samples ranging from pharmaceuticals to diesel emissions.
The embedded FTIR of acetone was recorded as a thin film using a PE1605 FTIR. The xyz files were calculated from output by Gaussian90 run on a Convex 3400 using a program (Vibread.exe) by Prof P. Lahti.
- All modern instruments are Fourier Transform instruments.

- In all transmission experiments radiation from a source is directed through the sample to a detector.
The measurement of the type and amount of light transmitted by the sample gives information about the structure of the molecules comprising the sample.
In the IR region of the electromagnetic spectrum, the absorption of radiation by a sample is due to changes in the vibrational energy states of a molecule.
CARBON DIOXIDE VIBRATIONS

(A) SYM. STRETCH

(B) ASYM. STRETCH

(C) BENDING (2)
The pattern of absorption as a function of wavelength is called an IR spectrum.
THE ABSORPTION PROCESS

RADIATION BEAM

ABSORPTION

FREQUENCY
To obtain an IR spectrum, the sample must be placed in a “container” or cell that is transparent in the IR region of the spectrum.

Sodium chloride or salt plates are a common means of placing the sample in the light beam of the instrument.
IR transparent Salt Plates
These plates are made of salt and must be stored in a water free environment such as the dessicator shown here.
Dessicator

Water-free Environment for Water-sensitive Salt Plates.
The plates must also be handled with gloves to avoid contact of the plate with moisture from one’s hands.
To run an IR spectrum of a liquid sample, a drop or two of the liquid sample is applied to a salt plate.
A second salt plate is placed on top of the first one such that the liquid forms a thin film “sandwiched” between the two plates.
The two plates are then secured in a sample holder that is compatible with the particular instrument being used.
- The cell holder is then placed in the beam of the instrument.
The light beam traverses the sample compartment, as illustrated by the red line.
Light Path
(shown by red line)
The sample is then scanned by the instrument utilizing predesignated parameters.

A relevant background scan should already have been taken.
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- A satisfactory spectrum has well defined peaks—but not so intense as to cause flattening on the bottom of the peaks.

- Major peaks can be labeled using the peak function of the software
Well-defined peaks are labeled with the Wavenumbers of the Absorption Maxima.
The spectrum can then be printed using the print function of the software.
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- A sample of a printout of an IR spectrum.
Sample of a printout of an IR spectrum.
The salt plates are cleaned by rinsing into a waste container with a suitable organic solvent—commonly cyclohexane.

NEVER WATER!
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CYCLOHEXANE
Solvent
Cloudy plates must be polished to return them to a transparent condition.

To polish cloudy windows, rotate salt plate on polishing cloth.
The clean plates and cell holder are stored in the moisture free atmosphere of a dessicator.