$$I(k)=\int_{\infty}^{0}[I(\Delta d)-I(\infty)]\cos(2\Pi k\Delta d)d\Delta d$$

FOURIER TRANSFORM INFRARED SPECTROSCOPY (FTIR)

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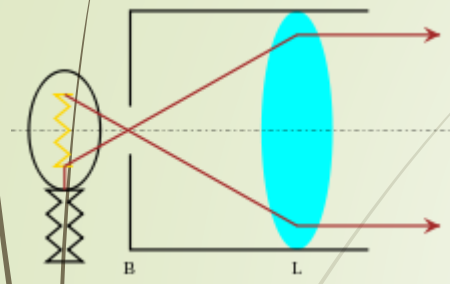
What is FTIR spectroscopy?

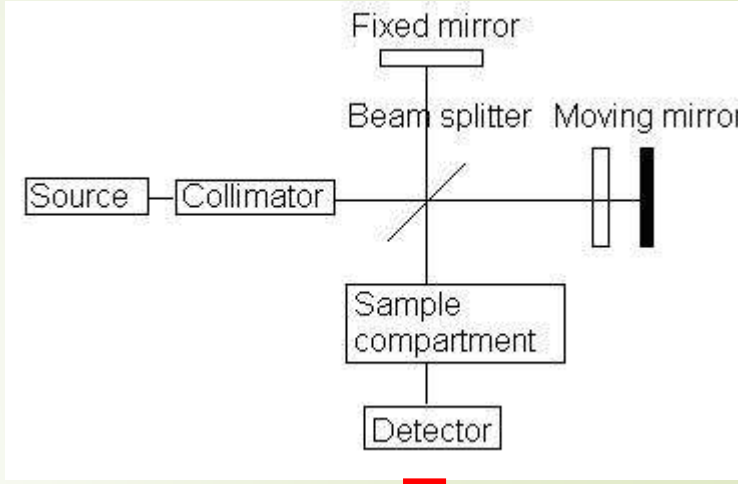


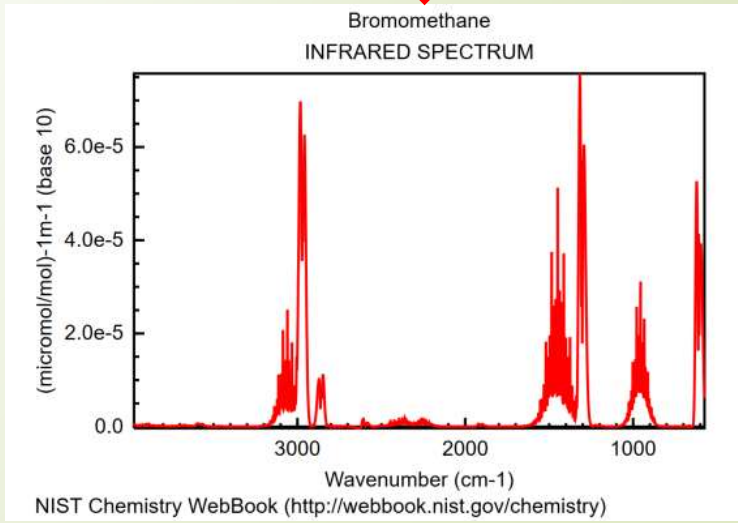
Infrared (IR) Spectrometer:

- IR light source is directed through a collimator, through a sample compartment and into a detector.
- Molecules in the sample absorb different wavelengths of the IR radiation.
- The unabsorbed wavelengths pass through the sample to the detector.
- The light received at the detector is converted to a digital signal.

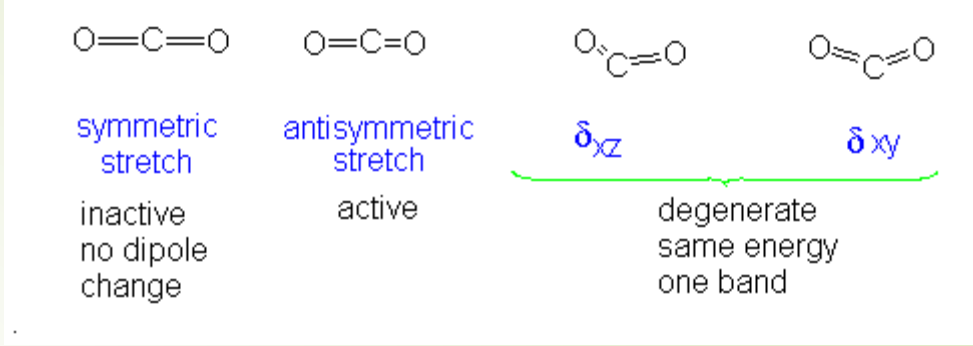
Fourier Transform (FT):

- The digital signal is converted mathematically (by Fourier Transform) to absorption or transmittance data that is plotted as a function of wavelength.
- The result is an "FTIR spectrum".



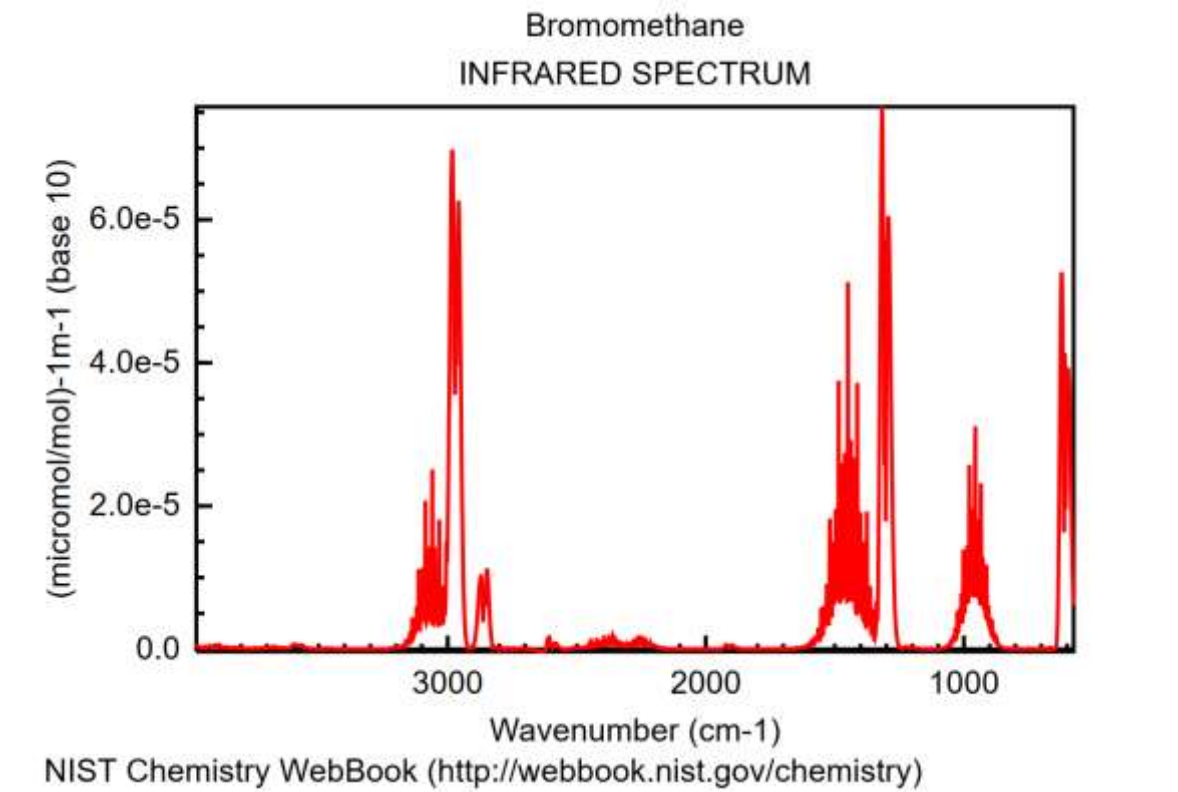


Principals of FTIR



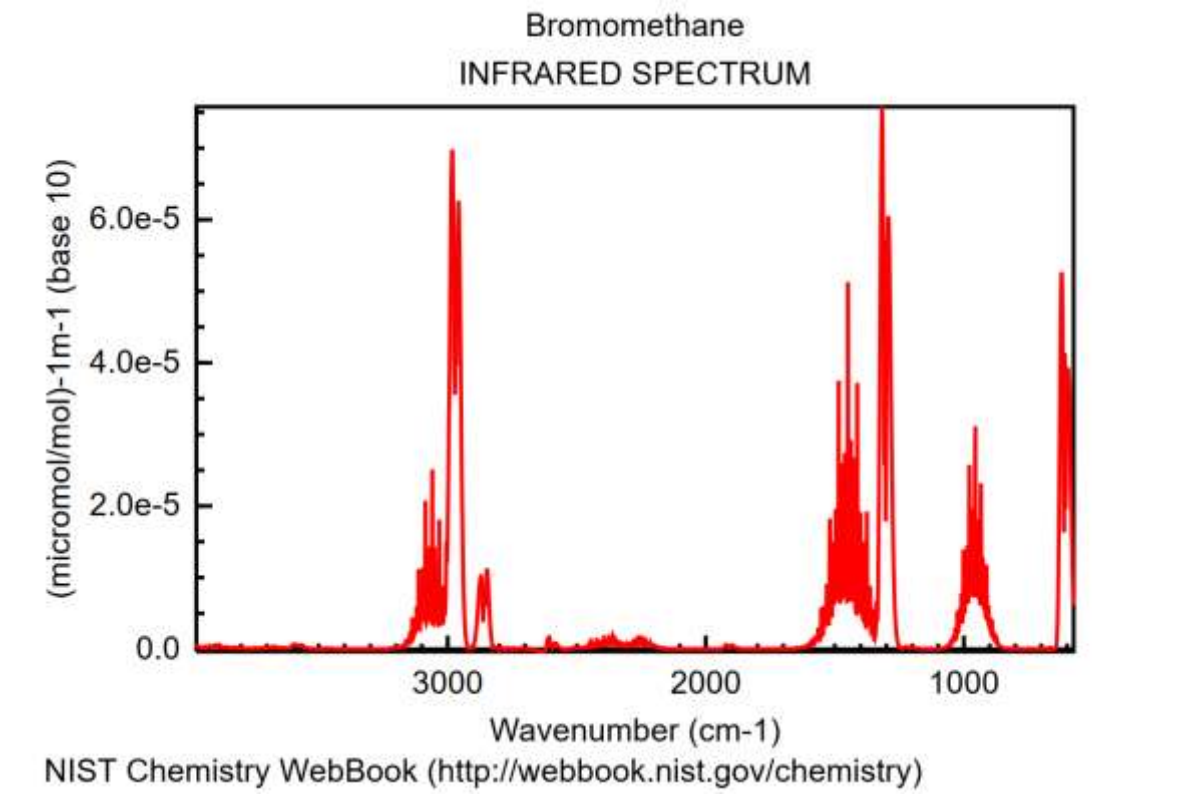
- The region for FTIR is typically 4000 - 400 cm^{-1}, and most organics and inorganics are IR active within this range.
- IR active molecules are those which experience a change in dipole moment when exposed to IR radiation.
- A change in dipole moment occurs through molecular rotations or "vibrations" (stretches or bends) in various ways.
- The amount of energy associated with each "vibration" corresponds to the IR wavelengths absorbed.
- NOTE: H_2, O_2, N_2, Cl_2 and all homonuclear diatomic molecules cannot be detected. (CO_2 is symmetrical, yet IR active because it has more than 2 atoms.)

FTIR spectrum



- **Each molecule has a unique IR spectrum ("signature" or "fingerprint").**
- Intensity of peaks relates directly to concentration in the sample compartment.
- The wavelength bands absorbed indicate which functional groups are present in the sample.
- Interferences in the spectra from different molecules that absorb at the same wavelengths (overlapping) can be resolved.

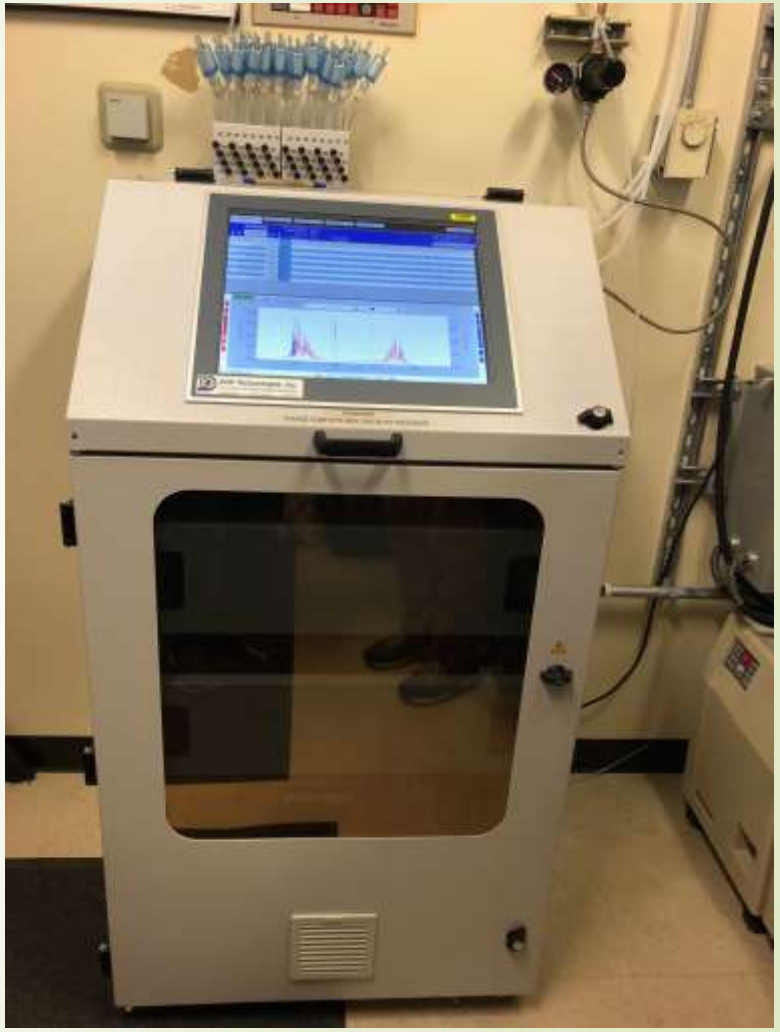
FTIR Capabilities and Applications



- FTIR takes simultaneous measurements of wavelengths, and can detect multiple gases in a mixture, simultaneously.
- Internal computer compares sample to NIST/EPA library calibration spectra for over 5,000 gas references.
- **FTIR can identify unknown gases!**
- **FTIR can quantify multiple gases simultaneously, from a single sample!**
- LDL's are typically below the ACGIH -TLV's at the ppb level (Phosphine, Arsine, Silane, Germane, Diborane, OM decomposition by-products, etc.).
- Some instruments will highlight unknowns, if a match is not found in the current library.
- Portable FTIR instruments can identify unknown sources of odors or fugitive toxic gases.

FTIR at NREL

- NREL currently uses the Vertex tape system to monitor hydrides.
- FTIR is being evaluated for use with OM's, inorganic acids, and as a back up for some hydrides, because of it's flexibility, speed, and ability to identify unknowns.
- Germane monitoring by tape technology takes up to 252 seconds to get a result.
- Response time using FTIR technology typically takes ~10 seconds.
- A single FTIR instrument can analyze for multiple chemical spectra at each monitoring point (up to 20 selections per point).



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