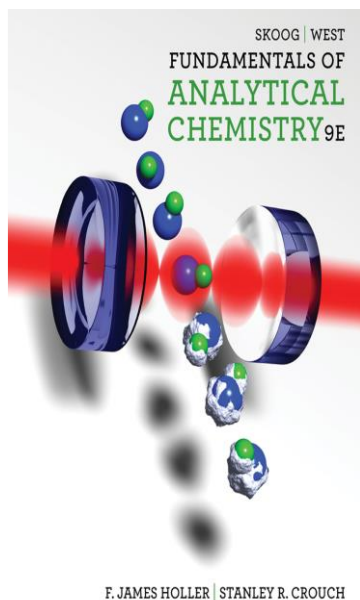
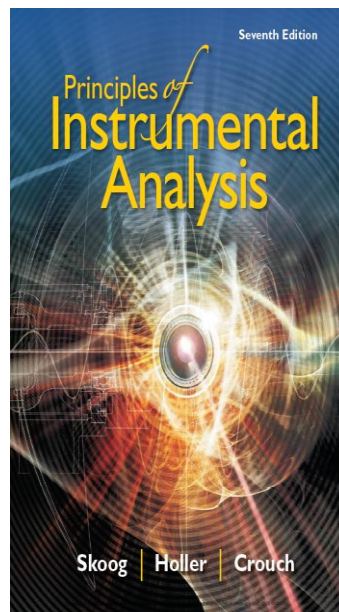


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ATAKOL's  
lecture notes

1. Skoog, D.A., West, D.M., Holler, J.F., Crouch, S.R. 2013. Fundamentals of Analytical Chemistry (9E). Cengage Learning, Belmont, USA.
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**Introduction to IR Spectroscopy,  
Principles and Applications,  
FTIR Devices**

# Infrared Absorption Spectroscopy

- Infrared spectroscopy is a powerful tool for identifying pure organic and inorganic compounds because, with the exception of a few homonuclear molecules such as  $O_2$ ,  $N_2$ , and  $Cl_2$ , all molecular species absorb infrared radiation.
- In addition, with the exception of chiral molecules in the crystalline state, every molecular compound has a unique infrared absorption spectrum.
- Therefore, an exact match between the spectrum of a compound of known structure and the spectrum of an analyte unambiguously identifies the analyte.
- Infrared spectroscopy is a less satisfactory tool for quantitative analyses than its ultraviolet and visible counterparts because of lower sensitivity and frequent deviations from Beer's law. Additionally, infrared absorbance measurements are considerably less precise.

# Infrared Absorption Spectra

- The energy of infrared radiation can excite vibrational and rotational transitions, but it is insufficient to excite electronic transitions.
- Infrared spectra exhibit narrow, closely spaced absorption peaks resulting from transitions among the various vibrational quantum levels.
- Variations in rotational levels may also give rise to a series of peaks for each vibrational state.
- With liquid or solid samples, however, rotation is often hindered or prevented, and the effects of these small energy differences are not detected. Thus, a typical infrared spectrum for a liquid consists of a series of vibrational bands.

- The number of ways a molecule can vibrate is related to the number of atoms, and thus the number of bonds, it contains. For even a simple molecule, the number of possible vibrations is large.
- Infrared absorption occurs not only with organic molecules but also with covalently bonded metal complexes, which are generally active in the longer-wavelength infrared region
- Infrared studies have provided important information about complex metal ions

# Instruments for Infrared Spectrometry

- Three types of infrared instruments are found in modern laboratories;
  - Dispersive spectrometers (spectrophotometers),
  - Fourier transform spectrometers, and
  - Filter photometers
- The first two are used for obtaining complete spectra for qualitative identification, while filter photometers are designed for quantitative work.
- Fourier transform and filter instruments are nondispersive in the sense that neither uses a grating or prism to disperse radiation into its component wavelengths.

# *Dispersive Spectrometers*

- With one difference, dispersive infrared instruments are similar in general design to the double-beam spectrophotometers.
- The difference lies in the location of the cell compartment with respect to the monochromator. In ultraviolet/visible instruments, cells are always located between the monochromator and the detector in order to avoid photochemical decomposition, which may occur if samples are exposed to the full power of an ultraviolet or visible source.
- Infrared radiation, in contrast, is not sufficiently energetic to bring about photodecomposition; thus, the cell compartment can be located between the source and the monochromator.
- This arrangement is advantageous because any scattered radiation generated in the cell compartment is largely removed by the monochromator.
- Infrared sources are heated solids rather than deuterium or tungsten lamps, infrared gratings are much coarser than those required for ultraviolet/visible radiation, and infrared detectors respond to heat rather than photons.
- In addition, the optical components of infrared instruments are constructed from polished solids, such as sodium chloride or potassium bromide.

## *Fourier Transform Spectrometers*

- Fourier transform infrared (FTIR) spectrometers offer the advantages of high sensitivity, resolution, and speed of data acquisition (data for an entire spectrum can be obtained in 1 s or less).
- FTIR spectrometers are commonplace, having replaced older, dispersive instruments in most laboratories.
- Fourier transform instruments contain no dispersing element, and all wavelengths are detected and measured simultaneously using a Michelson interferometer.
- In order to separate wavelengths, it is necessary to modulate the source signal and pass it through the sample in such a way that it can be recorded as an interferogram. The interferogram is subsequently decoded by Fourier transformation, a mathematical operation that is conveniently carried out by the computer, which is now an integral part of all spectrometers.



## *Filter Photometers*

- Infrared photometers designed to monitor the concentration of air pollutants, such as carbon monoxide, nitrobenzene, vinyl chloride, hydrogen cyanide, and pyridine.
- Interference filters, each designed for the determination of a specific pollutant, are available.
- There are also nondispersive spectrometers for monitoring gas streams for a single component.

## Qualitative applications of infrared spectrometry

- An infrared absorption spectrum, even one for a relatively simple compound, often contains a bewildering array of sharp peaks and minima. Peaks useful for the identification of functional groups are located in the shorter-wavelength region of the infrared (from about 2.5 to 8.5 mm), where the positions of the maxima are only slightly affected by the carbon skeleton of the molecule. This region of the spectrum thus abounds with information regarding the overall constitution of the molecule under investigation.
- Identifying functional groups in a molecule is seldom sufficient to positively identify the compound, and the entire spectrum from 2.5 to 15 mm must be compared with that of known compounds. Collections of spectra are available for this purpose.

# Quantitative Infrared Spectrometry

- Quantitative infrared absorption methods differ somewhat from their ultraviolet and visible counterparts because of the greater complexity of the spectra, the narrowness of the absorption bands, and the capabilities of the instruments available for measurements in this spectral region.