Infrared Spectroscopy Application in Pharmaceutical and Chemical Industries

Abstract:

The pharmaceutical and chemical industries deal with a wide variety of raw materials (excipients) and finished products, involving complex and diverse production processes. Many pharmaceuticals exhibit either complex chemical structures or minimal chemical differences among them, making conventional methods such as color reactions, precipitation, crystallization, or UV-VIS often insufficient for adequate differentiation. Infrared spectroscopy, with its high specificity, is a widely employed method in the qualitative analysis of organic compounds. In pharmaceutical inspection, infrared spectroscopy is frequently used in conjunction with other analytical methods, serving as a crucial means of identifying organic drugs.

Keywords:

Infrared spectroscopy, pharmaceutical and chemical industry, quality inspection

Principle:

Infrared spectroscopy utilizes the selective absorption of electromagnetic radiation by substances in the infrared spectrum to determine their molecular structure, achieving the qualitative identification of compounds.

Experimental Conditions:

Instrument and Accessories:

FTIR-7600: Fourier Transform Infrared Spectrometer
Solid testing accessories: Pellet press
Pellet molds
Agate mortar ϕ=60mm
Infrared drying oven (temperature-controlled)
Potassium bromide (spectroscopic grade)
Thin film testing accessories: Fixed liquid cell ϕ=32mm
Detachable liquid cell ϕ=25mm
Single-ATR accessories: ZnSe crystal with 45° angle of incidence

Ge crystal with 45° angle of incidence

Sample Preparation:

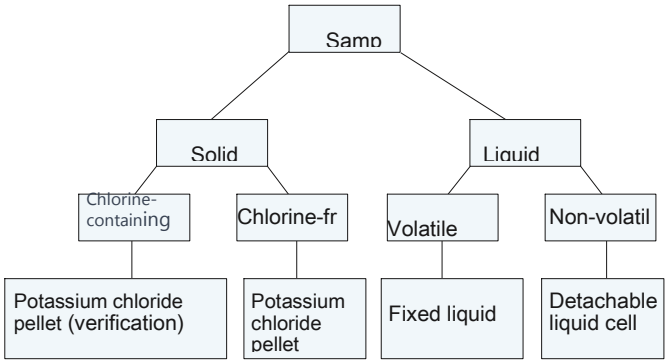

Chart 1 : Selection of Sample Preparation Method

Pellet Method: Mix the dried sample with potassium bromide (for chlorine-containing samples, ensure consistency with the potassium chloride pellet spectrum before using potassium bromide) in a ratio of about 1:200, grind evenly, take an appropriate amount, place it in the pellet mold, and make a pellet on the pellet press for testing.

Liquid Film Method: For volatile liquid samples (such as ethanol), take an appropriate amount with a glass syringe and inject it into the fixed liquid cell (ensure no air bubbles in the middle position of the window). For non-volatile samples (such as glycerol), use a capillary to drop an appropriate amount onto the middle position of the potassium bromide window, cover it with another potassium bromide window, rotate to form a film, fix the two windows, and then proceed with the testing.

Experimental Conditions:

Resolution: 4 cm^{-1}

Number of Scans: 32

Detector: DTGS

Example of Experimental Results

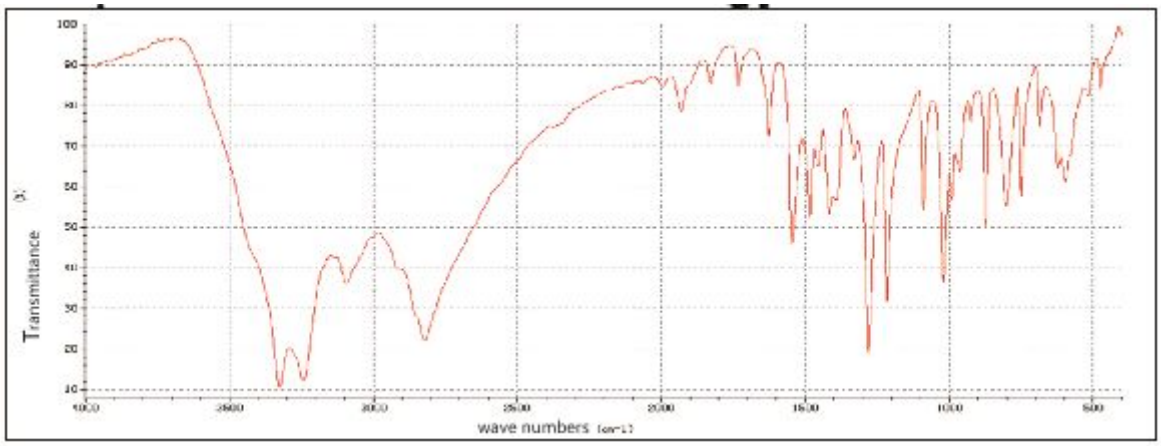

Chart 2: Vitamin B6 - Potassium Bromide Pellet Method Test Spectrum

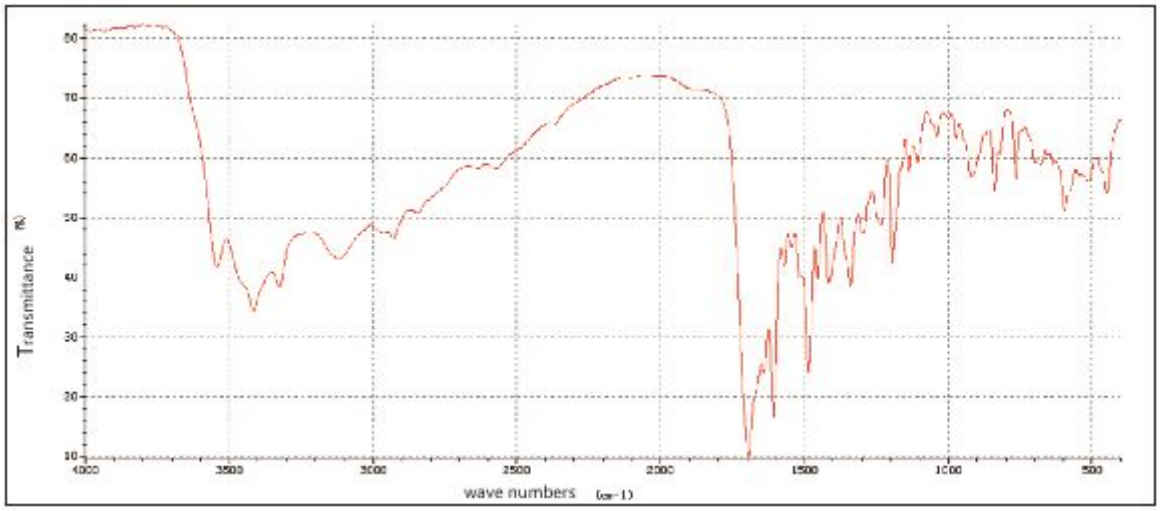

Chart 3: Folic Acid - Potassium Bromide Pellet Method Test Spectrum

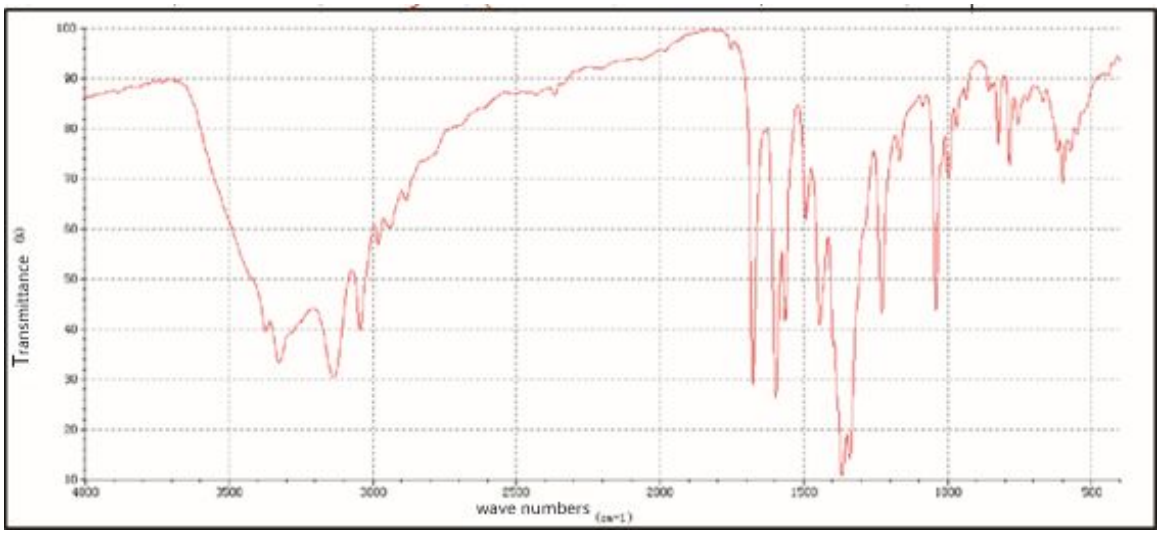

Chart 4 :Nitrofurantoin - Potassium Bromide Pellet Method Test Spectrum

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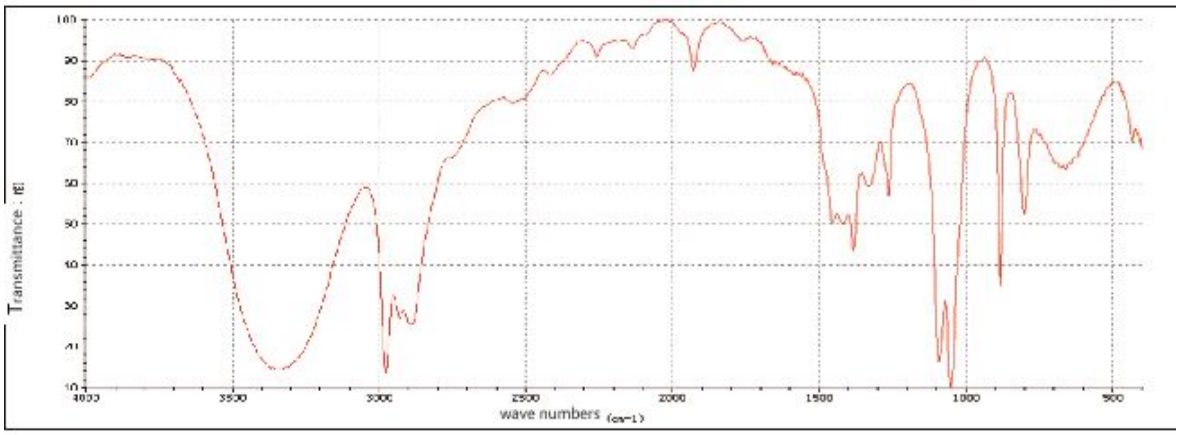

Chart 5: Ethanol - Fixed Liquid Cell Test Spectrum

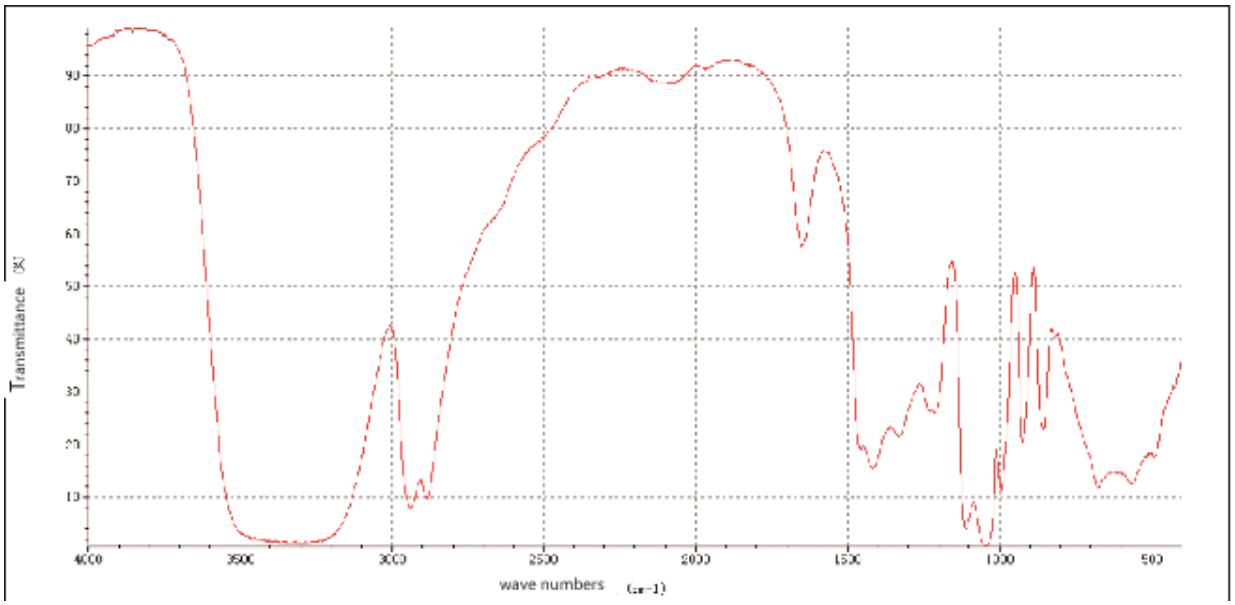

Chart 6: Glycerol - Detachable Liquid Cell Test Spectrum

The ATR method can be used for both solid and liquid sample analysis, eliminating the need for sample preparation. It allows for the quick analysis of multiple samples in a short period. The test spectra, after ATR correction, can be compared with spectra recorded in the "Infrared Spectra Collection of Drugs."

Conclusion:

The use of the ATR method for testing pharmaceutical packaging materials eliminates the need for sample preparation, allowing for in-situ analysis. This method, particularly advantageous in interface solid film testing, provides a simple and reliable way to qualitatively test pharmaceutical packaging materials. Infrared spectroscopy using ATR accessories is an ideal method for identifying pharmaceutical packaging materials.