**Lesson 6-7**

**Infrared spectrophotometry.**

Infrared spectroscopy (vibrational spectroscopy) is a branch of spectroscopy that studies the effect of infrared radiation on substances. When infrared rays pass through a substance, their molecules or certain fragments are excited. At this time, a decrease in the intensity of the beam passing through the test substance is recorded. However, the absorption of infrared rays does not occur in the entire spectrum, but only at wavelengths corresponding to the excitation of molecules. In this regard, wavelengths with a certain maximum absorption in the infrared spectrum indicate the presence of various functional groups in its composition. Therefore, infrared spectroscopy is widely used to study the structure of substances.

The nature of the absorption bands in the infrared field depends on the change in state and oscillating displacements of the nuclei that make up the molecule of a substance that absorbs electromagnetic radiation. Therefore, molecules with dipole states that change during the vibrational motion of their nucleus have the property of absorption in the infrared field. The scope of infrared spectroscopy is wider than that of UV. The IR spectrum uniquely characterizes the molecular structure of a substance. High specificity, objectivity of the results obtained, as well as the possibility of analyzing substances in crystalline form are among the advantages of IR spectroscopy. In single-beam or double-beam IR spectrophotometers, a mixture of a substance in paraffin oil is used to register IR spectra, or a substance is placed between plates of potassium bromide.

The infrared spectrum is a function of the emitted infrared radiation as a function of its frequency. Infrared spectroscopy is a valuable analytical method and is used in the study of various organic, inorganic and coordination substances. Infrared spectroscopy is a widely used analytical method based on the absorption of electromagnetic waves, and is successfully used in the study of the chemical structure of substances in pharmaceutical chemistry, for their identification and quantification. Using infrared spectroscopy, various functional groups in a molecule are quickly and accurately determined: carbonyl, carboxyl, hydroxyl, mono-, bi-, triamide and amino groups, etc. It is also possible to accurately identify parts of the molecule with unsaturated bonds (double and triple bonds, aromatic parts and etc.). Another advantage of infrared spectroscopy is the possibility of recording the spectra of substances in various states of aggregation - solid, liquid and gaseous. In addition, the interpretation of infrared spectra is easier than other spectroscopic methods.

IR spectroscopy is of exceptional importance for the identification of substances.

Basically, for the analysis of medicinal substances, the wavelength range of the spectrum from 4000 to 400 cm-1 is used.

The IR spectrum of a substance can be divided into three parts:

1. 3200-3600 cm-1 region of the spectrum - in this region, areas related to hydroxyl groups in the molecular composition of the substance are determined. Absorption bands in the regions 2993-2976 and 2851-2856 cm-1 in compounds containing methoxy groups in the molecule (characterized by the methoxy group OCH3).

2. The spectral regions 1500-1800 cm-1 are part of the characteristic absorption bands. In the region of 1700-1750 cm-1 of the spectrum, carbonyl (C=0) groups in the molecule are determined, which are an ester carbonyl (1700-1735 cm-1), a carbonyl of the δ-lactone cycle (1670-1720 cm-1) or can be carbonyl of the µ-lactone ring (1650-1780 cm-1). Depending on the different groups of natural compounds, there may be shifts in the characteristic absorption regions. For example, if the carbonyl group of the µ-lactone ring is conjugated to an exocyclic methylene double bond, its absorption band is determined in a relatively small region (1750-1770 cm-1).

The absorption bands of double bonds are in the fields of 1500-1690 cm-1 of the IR spectrum, the absorption bands of the aromatic system are in the fields of 1500-1630 cm-1, the absorption bands of the COO group are in the fields of 1700-1710 cm-1, C=C in the fields of 1620- 1680 cm-1 absorption bands.

The 1300-600 cm-1 regions of the IR spectrum are individual for each substance and are never the same. This area is different even in spatially isomeric compounds. This section of the IR spectrum is numerically individual for all substances and does not repeat.