Fourier transform infrared spectroscopy

Science, Chemistry

Introduction The range of Infrared region Is 12800- 10 cm-l. It can be divided into near-infrared region (12800 - 4000 crn-ll mid-infrared region (4000 - 200 crnl) and far-infrared region (50 ” 1000 cm-l). scientists have established various ways to utilize infrared light. Infrared absorption spectroscopy is the method which scientists use to determine the structures of molecules with the molecules' characteristic absorption of infrared radiation. Infrared spectrum is molecular vibrational spectrum.

When exposed to Infrared radiation, sample molecules selectively absorb radiation of pecific wavelengths which causes the change of dipole moment of sample molecules. Consequently, the vibrational energy levels of sample molecules transfer from ground state to excited state. The frequency of the absorption peak is determined by the vibrational energy gap. The number of absorption peaks is related to the number of vibrational freedom of the molecule. The intensity of absorption peaks is related to the change of dipole moment and the possibility of the transition of energy levels.

Therefore, by analyzing the infrared spectrum, one can readily obtain abundant structure information of a molecule. Most molecules are infrared active except for several homonuclear diatomic molecules such as 02, N2 and C12 due to the zero dipole change in the vibration and rotation of these molecules Concept: Fourier transform spectroscopy Is a less Intuitive way to obtain the same Information. Rather than shining a monochromatic beam of light at the sample, this technique shines a beam containing many frequencies of light at once, and measures how much of that beam Is absorbed by the sample.

Next, the beam Is modified to contain a different combination of frequencies, giving a second data point. This process is repeated many times. Afterwards, a computer takes all these data and works backwards to Infer what the absorption Is at each wavelength The beam described above is generated by starting with a broadband light source” one containing the full spectrum of wavelengths to be measured. The light shines into a Michelson interferometer” a certain configuration of mirrors, one of which is moved by a motor. As this mirror moves, each wavelength of light in the beam is periodically blocked. ransmitted, blocked, transmitted. by the Interferometer, due to wave interference. Different wavelengths are modulated at different rates, so that at each moment, the beam coming out of the interferometer has a different spectrum. Fourier Transform of Interferogram to Spectrum The interferogram is a function of time and the values outputted by this function of time are said to make up the time domain. The time domain Is Fourier transformed to get a frequency domain, which is deconvoluted to product a spectrum Step 1: The first step is sample preparation. The standard method to prepare solid sample for FTIR spectrometer is to use KBr.

About 2 mg of sample and 200 mg KBr re dried and ground. The particle size should be unified and less than two micrometers. Then, the mixture is squeezed to form transparent pellets which can be measured directly. For liquids with high boiling point or viscous solution, it can be added in between two NaCl pellets. Then the sample is fixed in the cell by skews and measured. For volatile liquid sample, it is dissolved in CS2 or CC14 to form 10% solution. Then the solution is injected into a liquid cell for measurement.

Gas sample needs to be measured in a gas cell with two KBr windows on each side. The gas cell should first be vacuumed.

Then the sample can be introduced to the gas cell for measurement. Step 2: The second step is getting a background spectrum by collecting an interferogram and its subsequent conversion to frequency data by inverse Fourier transform. We obtain the background spectrum because the solvent in which we place our sample will have traces of dissolved gases as well as solvent molecules that contribute information that are not our sample. The background spectrum will contain information about the species of gases and solvent molecules, which may then be subtracted away from our sample spectrum in order to gain nformation about Just the sample.

Figure 6 shows an example of an FTIR background spectrum. Figure 6. Background IR spectrum The background spectrum also takes into account several other factors related to the instrument performance, which includes information about the source, interferometer, detector, and the contribution of ambient water (note the two irregular groups of lines at about 3600 cm-l and about 1600 cm-l in Figure 6) and carbon dioxide (note the doublet at 2360 cm-l and sharp spike at 667 cm-l in Figure 6) present in the optical bench.

Step 3: Next, we collect a single-beam spectrum of he sample, which will contain absorption bands from the sample as well as the background (gaseous or solvent). Step 4: The ratio between the single-beam sample spectrum and the single beam background spectrum gives the spectrum of the sample (Figure 7). Advantages: Speed: Because all of the frequencies are

measured simultaneously, most measurements by FT-IR are made in a matter of seconds rather than several minutes.

This is sometimes referred to as the Felgett Advantage. Sensitivity: Sensitivity is dramatically improved with FT-IR for many reasons. The detectors employed are uch more sensitive, the optical throughput is much higher (referred to as the enable the coaddition of several scans in order to reduce the random measurement noise to any desired level (referred to as signal averaging). ? Mechanical Simplicity: The moving mirror in the interferometer is the only continuously moving part in the instrument. Thus, there is very little possibility of mechanical breakdown. Internally Calibrated: These instruments employ a HeNe laser as an internal wavelength calibration standard (referred to as the Connes Advantage). These instruments are self-calibratingand never need to be calibrated by the user.