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Until the mid-20th century, most organic compounds were distinguished from one another largely on the basis of simple physical and chemical properties. Knowledge of these properties, however, yields only superficial clues about a compound's molecular structure, and the determination of that structure was a complicated process (for large molecules at least) that involved careful analysis of several reaction pathways. Chemists had no way to see what molecules looked like, because molecules are so small that no device such as a microscope could be developed that would give a complete image of a molecular structure. One technique, X-ray crystallography, can give precise structural data for some molecules, but only those that can be obtained in solid, crystalline form. Normally, a full X-ray structure determination is a costly, time-consuming endeavour that is applied to only the most puzzling structures. Sufficient information to decipher a molecule's structure is much more easily obtained by the use of one or more spectroscopic techniques. Spectroscopy is a general term used for the instrumental processes by which information about molecular structure is obtained through careful analysis of the absorption, scattering, or emission of electromagnetic radiation by compounds. Electromagnetic radiation is the continuous spectrum of energy-bearing waves ranging from extremely short waves, such as high-energy X-rays (with wavelengths of about 10 nanometres [nm]), to very long, low-energy waves such as radio waves (with wavelengths of one metre [m] or more). Visible light, for example, is the range of electromagnetic radiation detectable by human vision, with wavelengths of roughly 400 to 700 nm. Objects appear coloured when they absorb visible light of certain wavelengths, and those absorbed wavelengths are consequently absent from light that passes from the coloured object to the eyes. Molecules are able to absorb light of certain wavelengths because the energy content of the absorbed light is the precise value needed to cause a molecule to be excited from one energy state to a higher one. The myriad energy levels in a molecule are said to be quantized because each one differs from another by a discrete, measurable energy value, just as each step in a stairway is a fixed height above, or below, all others. Thus, by measuring the wavelengths of the electromagnetic radiation absorbed by a molecule, it is possible to gain information about the various energy levels within it. This information can then be correlated with specific details of molecular structure. Instruments called spectrometers measure the wavelengths of light that are absorbed by molecules in various regions of the electromagnetic spectrum. The most important spectroscopic techniques for structure determination are ultraviolet and visible spectroscopy, infrared spectroscopy, and nuclear magnetic resonance spectroscopy. A fourth technique, termed mass spectrometry, does not depend on absorption of electromagnetic radiation, but it is valuable for the information it provides about the number and type of atoms present in a molecule. The following sections briefly describe the various applications of these techniques for organic compounds; for more information, see spectroscopy. Most organic compounds are transparent to the relatively high-energy radiation that constitutes the ultraviolet (200–400 nm) and visible (400–700 nm) portion of the electromagnetic spectrum, and consequently they appear colourless in solution. This is because the electrons in the *σ* bonds of organic molecules require wavelengths of even higher energy (such as those of X-rays) to excite them to the next higher accessible energy level. Electrons in *n* bonds, however, can be promoted to higher energy levels by ultraviolet and visible light, and UV-visible spectroscopy consequently provides useful structural information for molecules that contain *n* bonds. When multiple *n* bonds are separated from each other by intervening single bonds, they are said to be conjugated, ultraviolet-visible spectrum of azuleneEncyclopædia Britannica, Inc.The UV-visible spectrum of a molecule is dramatically affected by the presence of conjugation. As the number of conjugated *n* bonds increases, the UV-visible spectrum shows light absorption at a greater number of different wavelengths (i.e., the spectrum contains more absorption peaks), and light of longer wavelengths (and lower energy) is absorbed. The many individual peaks of UV-visible spectra normally coalesce to produce a continuous absorption spectrum, with some of the strongest individual absorption peaks appearing as sharp spikes. For example, the UV-visible spectrum of azulene, a molecule that contains five conjugated *n* bonds, shows a strong absorbance in the visible region of the electromagnetic spectrum, which correlates with its intense blue colour. Naturally occurring organic compounds that are highly coloured contain an extensive system of conjugated *n* bonds. The compound largely responsible for the bright orange colour of carrots, *β*-carotene, contains 11 conjugated *n* bonds. UV-visible spectroscopy is especially informative for molecules that contain conjugated *n* bonds. infrared spectrum of 5-hexene-2-oneEncyclopædia Britannica, Inc.In organic compounds, atoms are said to be bonded to each other through a *σ* bond when the two bonded atoms are held together by mutual attraction for the shared electron pair that lies between them. The two atoms do not remain static at a fixed distance from one another, however. They are free to vibrate back and forth about an average separation distance known as the average bond length. These movements are termed stretching vibrations. In addition, the bond axis (defined as the line directly joining two bonded atoms) of one bond may rock back and forth within the plane it shares with another bond or bend back and forth outside that plane. These movements are called bending vibrations. Both stretching and bending vibrations represent different energy levels of a molecule. These energy differences match the energies of wavelengths in the infrared region of the electromagnetic spectrum—i.e., those ranging from 2.5 to 15 micrometres (μm; 1 μm = 10–6m). An infrared spectrophotometer is an instrument that passes infrared light through an organic molecule and produces a spectrum that contains a plot of the amount of light transmitted on the vertical axis against the wavelength of infrared radiation on the horizontal axis. In infrared spectra the absorption peaks point downward because the vertical axis is the percent transmittance of the radiation through the sample. Absorption of radiation lowers the percent transmittance value. Since all bonds in an organic molecule interact with infrared radiation, IR spectra provide a great deal of structural data. The stretching vibrations of strong carbon-hydrogen bonds cause the absorptions around 3.4 μm, with the sharp peak at 3.2 μm due to the hydrogen atom on the carbon-carbon double bond. The many bending vibrations of carbon-hydrogen bonds cause the complicated absorption pattern ranging from about 7 to 25 μm. This area of IR spectra is called the fingerprint region, because the absorption pattern is highly complex but unique to each organic structure. The stretching vibrations for both the carbon-carbon and carbon-oxygen double bonds are easily identified at 6.1 and 5.8 μm, respectively. Most of the functional groups have characteristic IR absorptions similar to those for carbon-oxygen and carbon-carbon double bonds. Infrared spectroscopy is therefore extremely useful for determining the types of functional groups present in organic molecules. Absorption of long-wavelength (1–5 m) low-energy radiation in the radio-frequency region of the electromagnetic spectrum is due to the atomic nuclei in a molecule. Many (but not all) atomic nuclei have a small magnetic field, which makes them behave somewhat like tiny bar magnets. When placed in a strong external magnetic field, such nuclei can assume different energy states; in the simplest case, two energy states are possible. In the lower energy state, the magnetic field of the nucleus is aligned with the external magnetic field, and, in the higher energy state, it is aligned against the field. The energy difference between the two levels depends on the strength of the external magnetic field. In modern NMR spectrometers, organic compounds are placed in magnetic fields ranging from about 1.4 to 18.0 teslas (T) and are irradiated with radio-frequency waves. For comparison, the Earth's magnetic field is about 0.00007 T. At a magnetic-field strength of 1.4 T, the energy difference between the lower and higher energy states of a 1H proton nucleus is only 0.024 J mol⁻¹. Electromagnetic radiation with a frequency of about 60 megahertz (MHz) can supply the energy needed to convert the lower energy state to the higher one. The energy difference between the magnetic energy levels of a nucleus is measured as an absorption peak, or a resonance. Because the energy of the absorbed radiation depends on the environment around the absorbing nucleus in a molecule, NMR spectroscopy provides the most structural information of all the spectroscopic techniques used in chemistry. Especially valuable are proton magnetic resonance spectroscopy, which measures the resonances due to energy absorption by hydrogen atoms in organic compounds, and carbon-13 magnetic resonance spectroscopy, which yields the resonances due to absorption by atoms of carbon-13 (13C), a naturally occurring isotope of carbon that contains six protons and seven neutrons.

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