

INFRARED AND RAMAN SPECTROSCOPY

Introduction:

Spectroscopy studies the interaction of radiated energy and matter. Different types of radiation can be used to study local structural environments of atoms in crystals, and therewith chemical and physical material properties.

1) Electromagnetic radiation

2) Elementary particles (e.g., electrons, neutrons, protons)

3) Atomic nuclei (e.g., alpha particles)

4) Ions

5) Ultrasonic waves

Various types of radiation differ in wavelength or frequency but are physically identical. When light interacts with a material, different processes can occur, reflection of light, transmission, scattering, absorption or fluorescence. All these processes take place when the incident radiation induces changes in energy levels, which can be of electronic, vibrational or nuclear nature.

An example for the scattering process is the interaction of sunlight with the atmosphere: Sunlight consists of all the colors of the electromagnetic spectrum: red, orange, yellow, green, blue, and violet. Different colors of light have different energies or wavelengths. Red light has a long wavelength and a lower energy, whereas blue light has a short wavelength and a higher energy. When the sunlight passes through the atmosphere the gas molecules in the atmosphere scatter the sunlight, which is breaking up into its parts. However, they scatter the higher-energy blue wavelengths more effectively than the red wavelengths, so the sky looks blue.

Energy differences between ground and excited energy levels cover a wide range of the **electromagnetic spectrum** from radio waves to gamma rays, a wide range of transitions, such as nuclear spin level transitions, vibrations of molecular groups or electron transitions.

Parameters and Units

Depending on the application energies, **wavelengths**, **frequencies**, or **wavenumbers** are used.

The **energy** E (in kJ/mol or eV) is related to frequency ν or wavelength λ according to the equation $E = h\nu = hc/\lambda$, where h is the Planck constant (6.626×10^{-34} Js) and c is the speed of light in vacuum.

Electromagnetic radiation can also be characterized by its **wavelength** λ with the base unit m, but typically expressed in μm or nm.

$$1 \mu\text{m} = 10^{-6} \text{ m} = 10^{-4} \text{ cm} = 10^{-3} \text{ mm} = 10^3 \text{ nm}$$

The **frequency** ν describes the number of oscillations of the electric (or magnetic) radiation vector per unit of time. The typical unit is oscillations per second (s^{-1}), or Hz.

Wavelength and frequency are correlated through the following equation:

$$\nu = c / \lambda,$$

With c as the speed of light, which in a vacuum is $c_0 = 2.99793 \times 10^{10} \text{ cm s}^{-1}$. For other materials it can be calculated with following equation:

$$c_n = c_0 / n,$$

where c_n is speed of light in medium, n is the refractive index of the medium.

Wavenumber describes the number of waves per unit length and is very important for IR spectroscopy. It is expressed in cm^{-1} . It is the inverse of the wavelength ($1/\lambda$) and is proportional to the frequency ν , with wavenumber = ν / c .

Source:

https://serc.carleton.edu/NAGTWorkshops/mineralogy/mineral_physics/raman_ir.html