Department of Medical and Biological Physics **Emission and absorption of electromagnetic waves by a substance**



Lecture 6



Atomic and molecular energy levels Types of spectra. Spectral apparatuses **Ultraviolet and infrared radiation** Luminescence. Chemiluminescence **Light absorption and scattering Photocolorimetry Photobiological processes**

Corpuscular and wave properties of light and elementary particles

- A photon is an elementary particle of light with wave properties
- Energy of light photon is equal to $E=hf=h(c/\lambda)$, where h is a Plank's constant, f is a frequency
- The motion of particles (electrons, neutrons and so on) can be considered as a wave process with wavelength

$$\lambda = \frac{h}{m \ v}$$

where m is the mass of a particle, *v* is velocity

The Bohr model

Niels Bohr put forward in 1913 a theory of hydrogen atom:

- An electron in an atom can circle the nucleus without losing energy only in certain specific orbits
- 2) When an electron jumps from one orbit to another orbit it emits or absorbs a photon of light.

$$E_1 - E_2 = hf$$



 The frequency of emission (or absorption) of hydrogen atom can be expressed as

$$f = \frac{c}{\lambda} = \frac{E_n - E_k}{h} = \frac{me^4}{8\varepsilon_0^2 h^3} - \frac{1}{n^2} - \frac{1}{k^2}$$
$$\frac{1}{\lambda} = R \quad \frac{1}{k^2} - \frac{1}{n^2}$$

where R is a Rydberg constant $R = 10973731.568508(65) m^{-1}$



The bases of quantum theory

- In modern quantum theory the charge of electron is allocated within atomic space forming electron cloud with varying density. The density of electron cloud at any point of atom is equal to the probability of the detection of electron at the certain point.
 - The motion of electron in an atom is characterized by 4 quantum numbers:
- Principal quantum number (n=1,2,3...)
- Orbital quantum number $(0 \le l \le n-1)$
- Magnetic quantum number $(l \le m_l \le l)$
- Spin quantum number (+1/2 or -1/2)



The principles of the distribution of electrons into energy levels

- <u>Pauly's principle</u>: There are no electrons in an atom with the same set of quantum numbers
- <u>Minimal energy principle</u>: The distribution of electrons in an atom conforms to minimal energy of an atom

Each electron is characterized by the unique set of quantum numbers The aggregate of electrons with the same principle quantum number form an atomic energy level Atomic energy levels and the principal emission series of hydrogen atom



rom Bohr mode

Lyman Series

(Ultraviolet)

 $\frac{1}{n_2^2} eV$

Balmer Serie

(Visible) 410.2 nm

434.1 nm

violet

Molecular energy levels

- In polyatomic molecules we can distinguish three types of motion:
- Electronic (the motion of electrons around a nucleus)
- Vibration (the vibration of nuclei)
- Rotation (the change of orientation of molecular parts in a space)

The energy of molecule is equal to $E = E_e + E_v + E_r$

 $E_e \sim 1 \ eV, \ E_v \sim 10^{-2} \ eV, \ E_r \sim 10^{-4} \ eV$



Spectra

Spectrum is a plot of any quantity as function of either wavelength (λ) or frequency (f)

- The types of spectra:
- Continuous and line spectra
- Absorption and emission spectra

Absorption lines of hydrogen







Emission Lines of hydrogen

 $6 \rightarrow 2 \ 5 \rightarrow 2 \qquad 4 \rightarrow 2 \qquad n=3 \rightarrow 2$



- n=1 (Ground State)

Spectral apparatuses

- Spectral apparatus is used to separate the electromagnetic radiation (within optical band) into its components (wavelengths or frequencies) or analyze this radiation
- The apparatuses used for the visual observation of spectra are called <u>spectroscopes</u>
- The apparatus with photographic detectors of spectra is called <u>spectrograph</u>, with photoelectric detectors of radiation is called <u>spectrometer</u>

General scheme of spectral apparatus



Optical spectrum Visible





- The region UV-C is the most dangerous for living organisms and causes a bactericidal effect.
- The regions UV-A and UV-B are used for vitamin D formation.

Mercury lamps

- The medical resources of UV radiation are mercury lamps
- There are two types of mercury lamps:
- <u>high-pressure lamp</u> (150÷ 400 millimeters of mercury) and
- <u>low-pressure lamp</u> (0,01÷1,0 millimeters of mercury)

The <u>high-pressure</u> mercury lamp (λ_{max} = 365 nm)



- There is an argon gas with mercury drops inside quartz lamp
 - a, b are electrodes,
 - B is a plate,
- c, d are rings,
- K is a switch,
- D is a throttle,
- C_1, C_2 are capacitors

The high potential difference between electrodes and rings cause at first glow discharge then arc discharge
 Mercury vaporizes and emits UV radiation



- Infrared radiation is used for heating, for the activation of the cellular processes under the action of the temperature gradient.
- The IR sources are heated bodies











Luminescence is a process of producing light without involving or generating heat that lasts over the optical vibration period



Simplified Jablonski Diagram

Characteristics of luminescence

• Stokes shift

• Quantum Yield

• Energy Yield

Stokes Shift



Wavelength

- Lumenescence spectrum and its peak shift to the higher wavelength region in comparison with the energy peak of absorbance.
- $E_{abs} = E_{non-radiating} + E_{flu}$

• Quantum Yield



• Energy Yield

$$W = \frac{energy \ emmitted}{energy \ absorbed}$$

Two types of luminescence:

Fluorescence (short-duration luminescence):

Emission involves a spin allowed transition (short excited state lifetime)

Phosphorescence (long-duration luminescence): Emission involves a spin forbidden transition

(long lived excited state).



Luminescence in medicine

- The green fluorescent protein (GFP) from jellyfish exhibits bright green fluorescence when exposed to light in the blue to UV range. It is widely used in fluorescent microscopy.
- Luminescence analysis is allows to detect the compounds in the concentrations about 10⁻¹⁰ M
- The bacterial and mycotic colonies are characterised by specific luminescence.
 This luminescence is used for diagnosing different diseases in dermatology.





Light absorption is a light energy transformation into other types of internal energy



Green colour of leaf is due to the absorption of blue and yellow/red light The photosynthetic pigments absorb much of the spectrum



The law of light absorption



 $I_{1} = I_{0}e$

The constant *a* is called *the absorption coefficient* **at the wavelength considered**.

Beer-Lambert law of light absorption

• For diluted solutions:

$$I_{l} = I_{0}e^{-\varepsilon_{1}cl}$$
 or $I_{l} = I_{0}10^{-\chi_{1}cl}$

where ε and χ are the absorptivity of the substance at the wavelength considered for the unit of substance concentration (the index of extinction).

Photocolorimetry

 is a method of determination of substance concentrations using the absorbance measurements.

 The devices for photocolorimetry are called photo colorimeters.

Photo colorimeter principle



The light-transmission factor (or solution transparency)

• is the ratio of the intensity of light transmitted through the sample (I) to the intensity of light incident on the sample (I_{θ})

 $\tau = \frac{I_l}{I_0}$

The absorbance (or optical density)

• is the logarithm of the inverse lighttransmission factor is called *an absorbance*

 $A = \log \frac{1}{\tau} = \mathcal{E}_1 cl$

Example. Determination of the tissue oxygenation coefficient

To estimate the concentration of HbO_2 and Hb in living tissues the absorbance is measured at two wavelengths (660 nm and 920 nm)



Tissue oxygenation coefficient

can be estimated as

$$pO_2 = \frac{[HbO_2]}{[HbO_2] + [Hb]}$$

The device for measuring the tissue oxygenation is **Oxymeter (oximeter)**





Light scattering by the turbid medium

- The phenomenon of the deviation of light from linear propagation in turbid medium is called the light scattering
- Two types of optical heterogeneities:
- 1) small foreign inclusions in homogeneous transparent substance (Tindall's phenomenon)
- 2) optical heterogeneities appeared in pure substance due to density fluctuations (molecular scattering). $I \approx \frac{1}{\lambda^4}$

The general law of decrease in light intensity due to the light absorption and light scattering

$$I_{l} = I_{0} \ 10^{-\mu l}$$

where μ is the loss coefficient, μ= χ+k,
k is the scattering coefficient.

Turbidimetry (nephelometry)

• is a method of measurement of scattered light for getting information about particle size and parameters of intermolecular interaction.

• The devices for nephelometry are called nephelometers.

Photobiological processes

• are that start with light absorption and result in a certain physiological reaction of an organism.

The positive photobiological processes

• vision,

- *photoperiodic response* (the regulation of daily and yearly living rhythms of animals with periodic effect of light and dark.
- vitamin D formation from its provitamins

The negative photobiological processes

- phototoxic effects:
- light injury of eyes and skin (lenticular opacity, erythema)
- bactericidal action of UV;
- • carcinogenic action of UV.
- photoallergic effects