X - rays

November 6, 2013

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Discovery

Wilhelm Conrad Roentgen

(1845-1923)

Discovery in 1895 November ->
publication in December ->
1896 January:* *Medical applications

(a)

Figure 4.10 Two radiographs taken by Röntgen. (a) The hand of Mrs. Röntgen. *(The Bettmann Archive/Bettmann Newsphotos.)* (b) Radiograph of a fully clothed man, showing not only the man's skeleton but also the keys in his pockets, the nails of his shoes, and the metal clasps of his garters. *(Deutsches Museum, Munchen.)*

(b)

Hungary: Device for Medical diagnostics TechnicalUniversity (Budapest) in 1896

First Nobel laurate in physics 1901

"in recognition of the extraordinary services he has rendered by the ***discovery of the remarkable rays*** *subsequently named after him".*

(Medicine: Adolf von Behring - *for his work on serum therapy, especially its application against diphtheria*

Chemistry: Jacobus Henricus van 't Hoff - *chemical dynamics and osmotic pressure in solutions*)

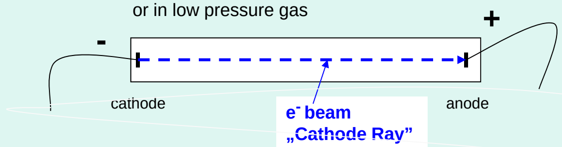
The „Golden Years" of physics

1895: X-radiation – Röntgen
1896: radioactivity – Becquerel
1897: electron – J. J. Thomson
1898: Radium – Pierre and Mme Curie

Basic experimental device: Cathode Ray Tube – CRT

- discovery of X-rays
- discovery of the electron

Glass tube with two electrodes in vacuum
or in low pressure gas



Electrons emitted by the cathode due to field emission, and accelerated by the positive potential of the anode.

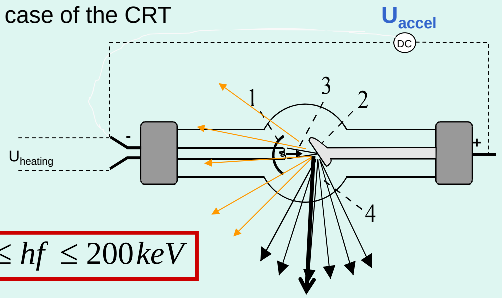
Later: cathodes were heated by an electric circuit to emit more electrons

Roentgen's observations

- cathode ray generates radiation in the wall of the tube
- the radiation is similar to UV light – induces fluorescence
- but is of much higher penetration
- is not reflected and refracted like light

X-ray Tube: X-ray source for Medical Diagnostics

a special case of the CRT

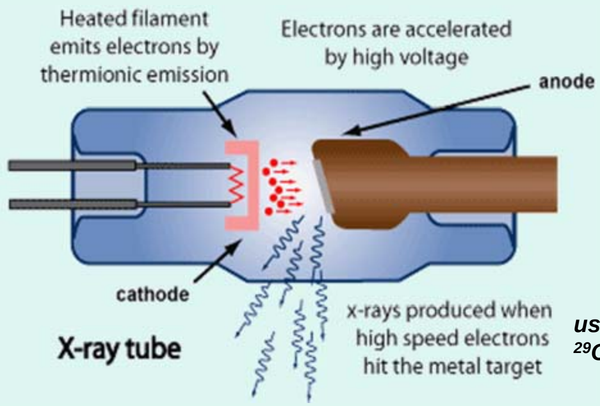


1. Heated cathode
2. Anode
3. Electron beam
4. X-radiation

$$\boxed{20keV \leq hf \leq 200keV}$$

Higher photon energies required for tumor therapy are produced by particle accelerators

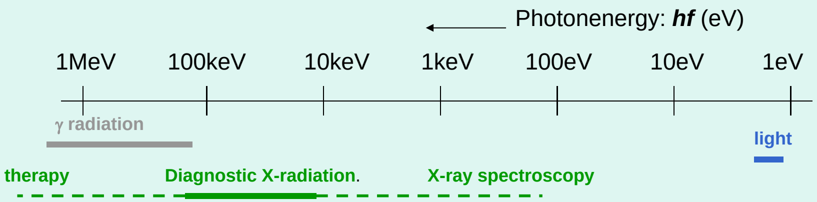
More detailed schematics



usual target metals:
^{29}Cu, ^{42}Mo, ^{74}W, ^{78}Pt

X-ray production is of very low efficiency << 1%

X-rays in the spectrum of elecromagnetic radiations



X-radiation: *electromagnetic radiation of high photonenergy as compared to light*

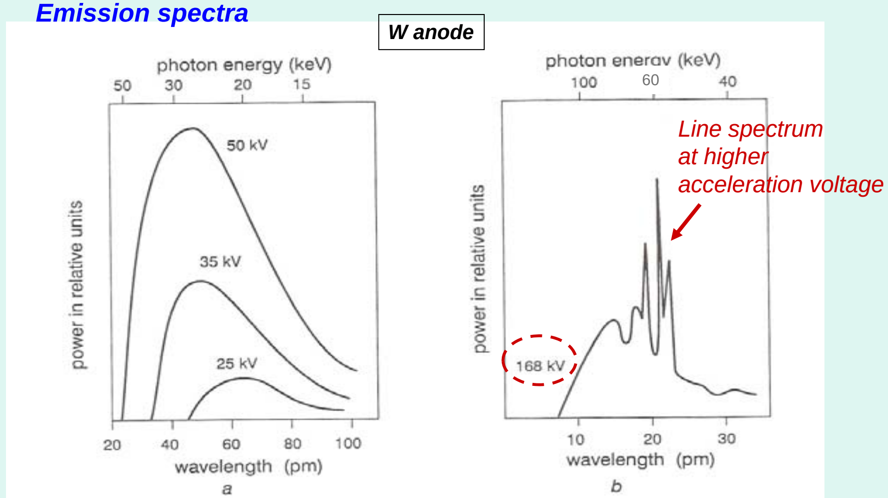
Dual nature: photon or wave –models?

Wave- concept : X – ray diffraction and interference

Photon concept: absorption of the energy of X-radiation

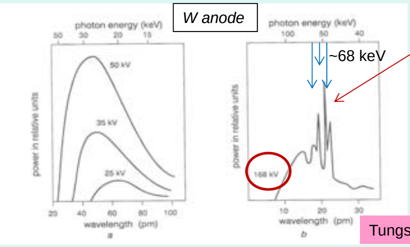
The radiation emitted by the X-ray Tube

Emission spectra



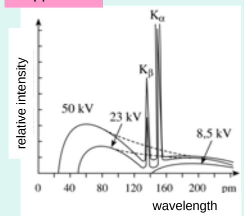
Spectra of Braking Radiation ***Lines of Characteristic X Radiation***

1.Characteristic radiation – X-ray luminescence
Spectra



***Line spectrum** appears superimposed on the continuous Bremsstrahlung at higher acceleration voltages*

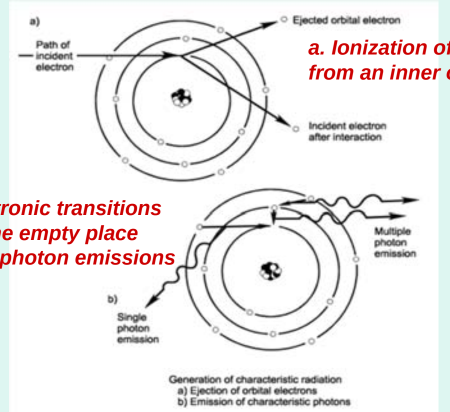
The photonenergies of the emission lines are characteristic for the material of the anode



The photonenergies of the lines must be related to the electronic orbital energies of the target (anode) material

and do not depend on the accelerating voltage

Characteristic radiation – X-ray luminescence
Mechanism of generation

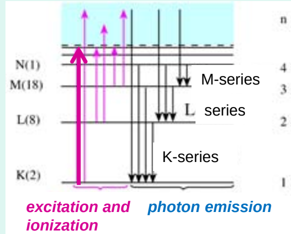


a. Ionization of electron from an inner orbital

$\Delta E = hf$

b. Electronic transitions to fill the empty place lead to photon emissions

Example: electronic orbitals of the ***Cu*** atom with 29 electrons



K-edge : ionization energy from the K-shell

transitions terminating in the K shell give rise to the K-lines, those terminating in the L shell produce the L -lines, and so on.

The energy differences between inner shells grow with Z (the number of electrons in the atom)

Ionization energies from the K level: „K-edge"

Al(13)	1.6 keV
Fe(26)	7.1 keV
Cu(29)	9.0 keV
Zn(30)	9.7 keV
Mo(42)	19.9 keV
W(74)	69.5 keV

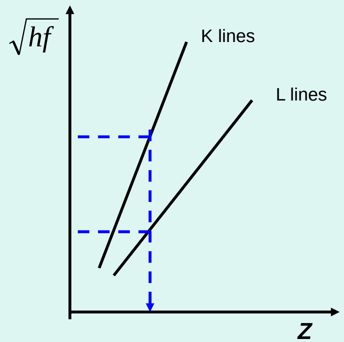
atomic number: Z

The orbital energy differences are large between inner orbitals of atoms of high atomic number

Practical applications of Characteristic X-radiation

1. ***Chemical analysis***

- *from minute amounts*
- *sample plays the role of an anode*



qualitative analysis:

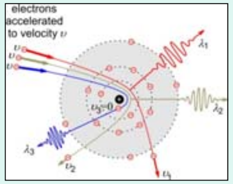
photon energies of spectral lines define the atomic number of the sample

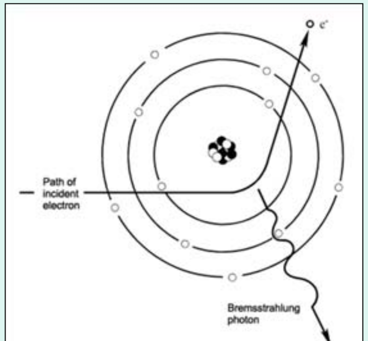
Analysis in criminology

2. Braking radiation - Bremsstrahlung

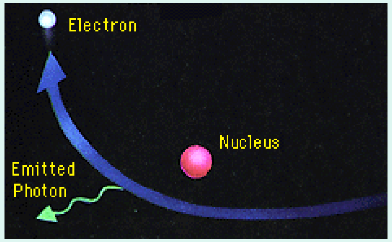
Mechanism

***Charged particles** accelerated to high kinetic energy are **decelerated** in a target material. Some steps of deceleration produces X-ray photons on the expense of the kinetic energy.*





Generation of Bremsstrahlung



Braking Radiation - Bremsstrahlung

Emission Spectra

1. Spectrum is ***continuous: all λ and hf***
- ***above** a certain wavelength*
- ***below** a certain photonenergy*

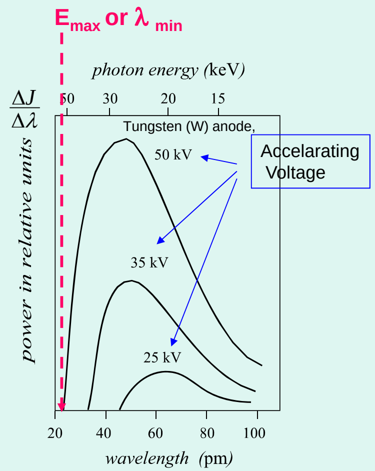
$$\boxed{hf_{max} = h\frac{c}{\lambda_{min}} = q_{electron}U_{accel}}$$

Planck's constant

Duane-Hunt law

$$\boxed{\lambda_{min} = \frac{hc}{q_e}\frac{1}{U_a}}$$

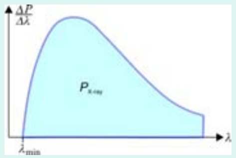
Increased accelerating voltage broadens the spectrum towards shorter wavelengths (higher photonenergies)



Braking Radiation - Bremsstrahlung

Emission Spectra

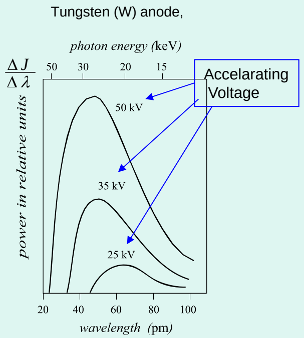
2. *The total emitted power increases with the voltage and current intensity*



$$\boxed{P_{total} = const_{Xray} \cdot U_{anode}^{\;2} \cdot Z_{anode} \cdot I_e}$$

$$const \approx 1.1 \cdot 10^{-9}\mathrm{V}^{-1}$$

empirical constant

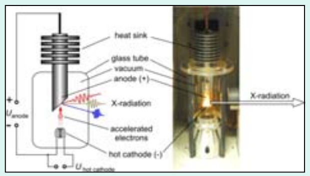


$$P_{total} \approx U^2$$

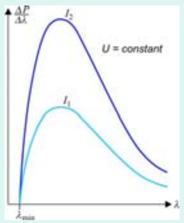
$$P_{total} \approx I$$

Adjustable parameters of X-ray tube

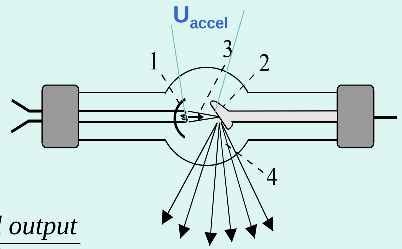
Different effects!



3. *The electron-current intensity does not change the spectrum*



Estimating the radiation yield of the X-ray Tube - Bremsstrahlung



$$efficiency\,(\eta) = \frac{useful\ output}{total\ input}$$

~$10^{-9}\mathrm{V}^{-1}$ 100 kV Z_w=74

$$\eta = \frac{P_{radiation}}{P_{electric}} = \frac{c_{Xray}U^2 I\, Z}{U\ I} = c_{Xray}U\ Z$$

$$\boxed{\eta \approx 0.008}$$

The radiation yield is very low < 1%
Great heat loss!

Increasing U increases the radiation efficiency ⟷ ***BUT changes the spectrum!***

How X-ray tubes really look like

X-ray production is of very low efficiency << 1%
high heat generation → cooling (circulating oil)
→ rotating anode

Basics of X-ray diagnostics

Diagnostic applications are based on the contrast in the image based on the ***variety of absorption in various tissues***

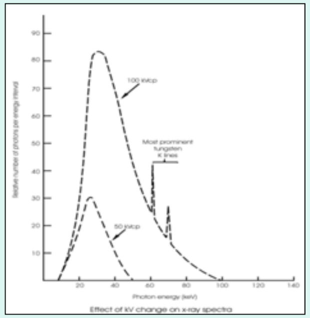
$$J = J_0 e^{-\mu x} = J_0 e^{-\mu_m \rho x}$$

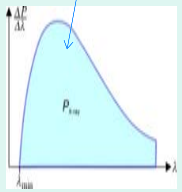
depends also on the photonenergy of X-rays

$J_0 \rightarrow \boxed{\mu_m \ \rho} \rightarrow J$

μ attenuation coefficient
μ_m mass attenuation coefficient
ρ density of absorber

$$J\left[\frac{W}{m^2}\right] = \frac{P_{total}[W]}{A[m^2]}$$



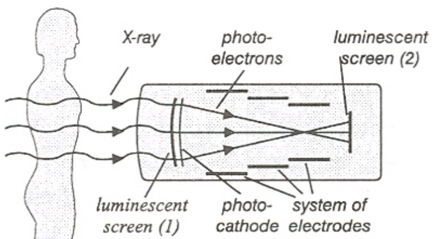


Sharp lines of characteristic radiation can be neglected in the contrast based on the variety of μ

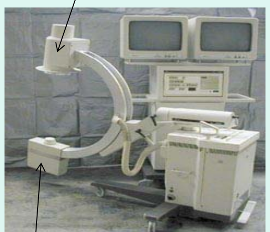
Diagnostics is based on the absorption of Bremsstrahlung

Diagnostics is based on the absorption of X-rays of ionizing radiation

Radiation hazard !



X-ray image amplifier
- *to decrease the illuminating X-ray intensity (to 10-20%)*
- *to convert the image into optical image → digitalization*



Mechanism of X-ray absorption in function of photonenergy

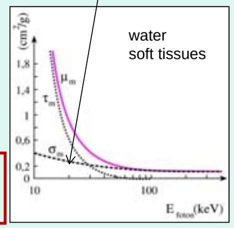
the range of the X-ray tube: 20 keV<hf< 200 keV

$$J = J_o e^{-\mu x} = J_o e^{-\mu_m \rho x}$$
$$\mu = \mu_m \rho$$
$$\mu_m = \tau_m + \sigma_m$$

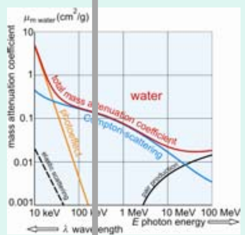
photoelectric effect is of highest probability, strongly depends on Z of absorber and on the photonenergy of X-rays

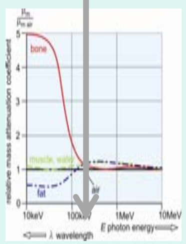
Compton effect
σ_m of water ~ constant~ 0.2cm²/g

$$\tau_m = const_1 * \lambda^3 Z^3 = const_2 * \frac{Z^3}{(hf)^3}$$



diagnostic range

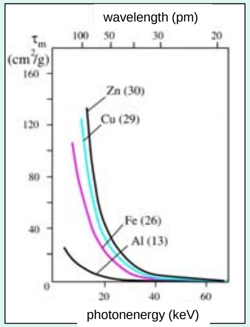




X-rays of low photonenergy are very well absorbed in the tissues

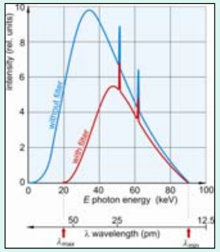
Practical acpects of X-ray diagnostics

1. Filtering the radiation - cutting off the photons of low energy → decreasing the radiation hazard



→

Using Al filter eliminates the photons <20 keV and partially absorbs at higher energies.



$$\boxed{\tau_m = const_1 * \lambda^3 Z^3 = const_2 * \frac{Z^3}{(hf)^3}}$$

materials of ***medium Z*** are good for filtering

Photons of low energy are not absorbed in the skin, but in the filter.

2. Using contrast materials – *positive and negative contrast of organs*

Zeff takes into account the atomic composition of the absorber

$$Z_{eff} = \sqrt[3]{\sum_{i=1}^{n} w_i Z_i^3}$$

molar ratio

$$\boxed{\begin{aligned} \tau_m &= const * \lambda^3 Z^3 \\ J &= J_o e^{-\mu x} = J_o e^{-(\tau_m + \sigma_m) * \rho * x} \end{aligned}}$$

material	Z_{eff}	ρ (g/cm3)
air	7,3	**$1,3 \cdot 10^{-3}$**
water	7,7	1
soft tissue	7,4	1
bone tissue	**13,8**	**1,7-2**

Contrast material filling the organ leads to

inreased absorption positive contrast or decreased absorption negative contrast

Positive contrast materials *(Iodine, Barium, etc.)*

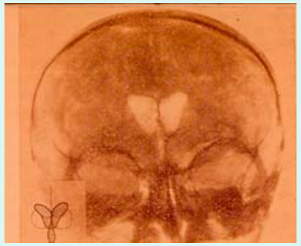
Z high → τ_m high → μ high

Negative contrast materials *(gases: air, CO_2, etc)*

ρ low → μ low

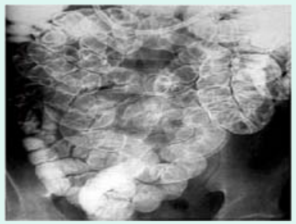
$$\boxed{\mu = \mu_m * \rho}$$

Bowels (positive contrast)



Air (negative contrast)

Large intestine (double contrast)



Small intestine (double contrast)

DSA *method - based on positive contrast*

Digital Subtraction Angiography

Image 1

(without *I* contrast)

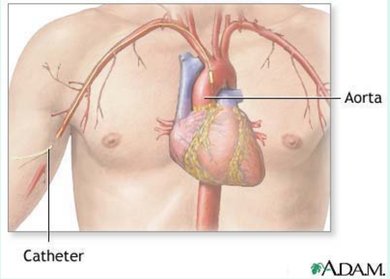
Image 2

(with contrast)

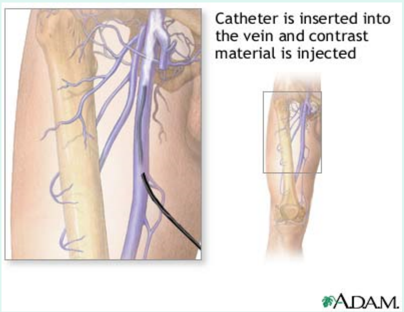
DSA image: subraction of Image1 from Image2

(contrast-native)

Cardiac arteriogram

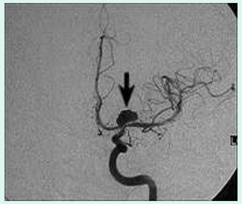


Considered as surgical intervention



Cerebral arteriograms

Normal frontal cerebral arteriogram

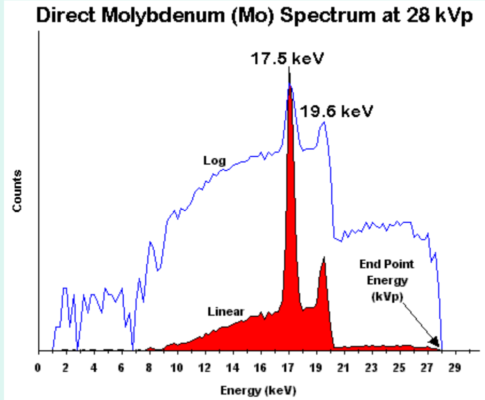


a large aneurysm arising from the left internal carotid artery in the brain.

Diagnostic application of characteristic radiation of Molibdenium

Mammography

low photonenergy, monochromatic (~17.5 keV) radiaton of Mo anode is absorbed in soft tissues with high probability



X-ray computed tomography yields 3D images
„driver in a car” -- discussed later

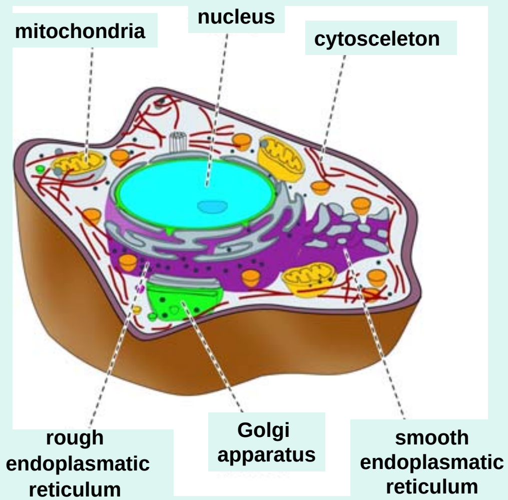
End of the topics of X-rays

New topics follow!

Considering matter as built up from a large number of atoms

The concept of Boltzmann-distribution

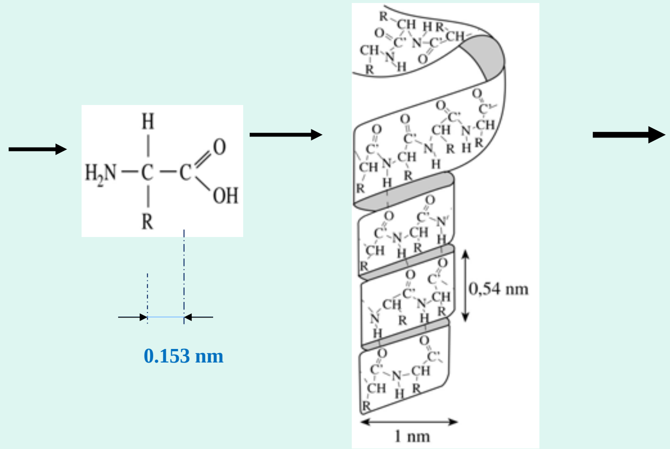
Cell: functional unit of biological materials



highly organized,
densely packed
system of interacting
ions,molecules
and macromolecules

Atoms | *Molecules* | *Macromolecules*

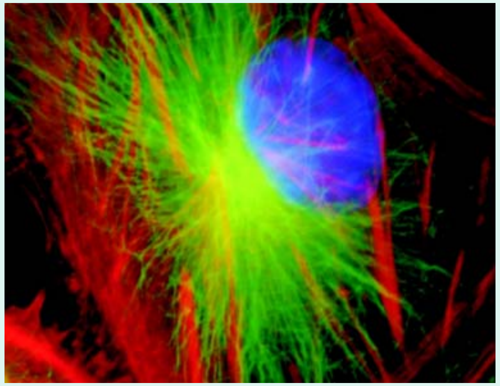
H
O
C
N
S
.
.
.



Hierarchy of bonds, bond energies, bond distances…..

Blue:nucleus

Red:actin filaments

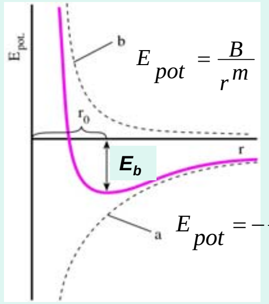


Green:microtubules

Until now: atomic view, energy minimum concept

Examples:

1. How bonds are formed



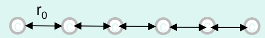
$$E_{pot} = \frac{B}{r^m}$$ repulsion

$m>n$

$$E_{pot} = -\frac{A}{r^n}$$ attraction

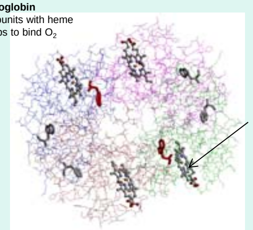
r= distance of two atoms forming the bond
r_o= bond distance
E_{bond}= bond energy

Atomic/molecular bond distances and binding energies E_b depend on the type of interactions (functions ***a*** and ***b***)



If many atoms – do they sit exactly at r_0 distances from each other all the time?

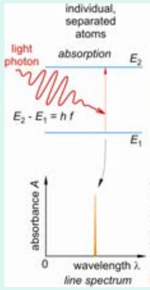
Hemoglobin
4 subunits with heme groups to bind O_2

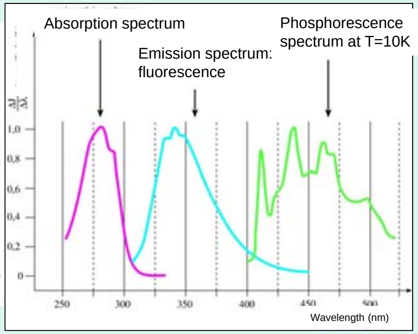


How does O_2 get through the protein to reach the heme?

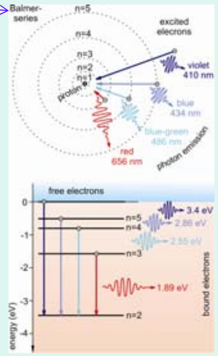
2. Photon absorption and emission

Light absorption and emission: Strictly quantized phenomena



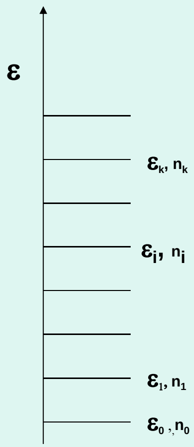


Spectra of tryptophan in a protein



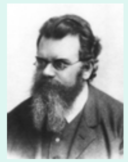
Why are the spectra of molecular electronic systems so broad? Is the transition energy not strictly defined by the electronic energy levels? Do not the electrons choose the transitions of energy minimum condition?

Boltzmann distribution



N distinguishable independent particles at thermal equilibrium, T≠ 0 in a closed system

ε_j possible energy status for one particle
n_j number of particles having ε_j energies



Ludwig Eduard Boltzmann
1844-1906, Austrian physicist

$$E = \sum_j n_j \varepsilon_j \qquad N = \sum_j n_j$$

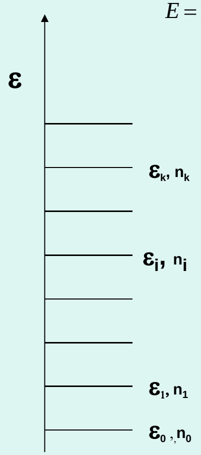
Boltzmann distribution function

$$\frac{n_k}{n_j} = e^{-\frac{\varepsilon_k - \varepsilon_j}{kT}} = e^{-\frac{\Delta\varepsilon}{kT}}$$

Boltzmann factor

Valid for any (j,k) combinations of energy levels

Boltzmann distribution - conclusions



$$E = \sum_j n_j \varepsilon_j \qquad N = \sum_j n_j$$

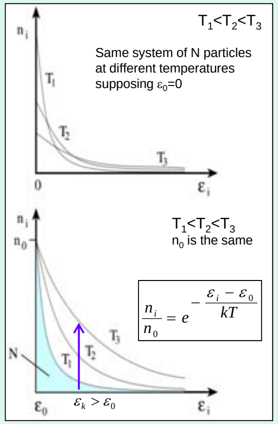
$$\frac{n_k}{n_j} = e^{-\frac{\varepsilon_k - \varepsilon_j}{kT}} = e^{-\frac{\Delta\varepsilon}{kT}}$$

Populations of potential energy states „distribution" of particles is given

$$\frac{n_i}{n_0} = e^{-\frac{\varepsilon_i - \varepsilon_0}{kT}} = e^{-\frac{\varepsilon_i}{kT}}$$

As the temperature is lowered, more and more particles are in the energy minimum state at T=0 all particles are there: $n_i=0$, $n_0=N$

At a given $\varepsilon_k > \varepsilon_0$ energy level, the relative population related to the energy minimum increases with the temperature



Boltzmann distribution - examples

1. Structural order ? – live matter at T=310 K

If many atoms – do they sit exactly at r_0 distances from each other all the time?
Is it possible that some bonds are even „broken" at T=310 K?

$$\boxed{\frac{n_{broken}}{n_{bound}} = e^{-\frac{\Delta\varepsilon}{kT}} \qquad \Delta\varepsilon = E_{bond}}$$

kT ~ 0.027 eV T=310 K, ***k***=1.38x10^{-23}JK^{-1} *Boltzmann constant*

$\boxed{kT \longleftrightarrow E_{bond}}$ **?**

electronvolt
1 eV= 23 kcal/mole ~
~ 100 kJ/mole

Classes of bonds – hierarchy of bond energies		E_{bond} (eV)	$e^{-\frac{\Delta\varepsilon}{kT}}$	n_{broken}
- Primary bonds: ionic, covalent, (metallic)		2 – 6	~ 0	none
- Secondary bonds:				
	H – bonds	~ 0.2		↓
	hydrophobic int.	~ 0.1		
	dipole int.	0.01 – 0.1		
	van der Waals (dispersion)	0.02	~ 0.5	many

e.g. how many broken H-bonds are in the dsDNA of the T7 bacteriophage at T= 300 K ?

$$\frac{n_{broken}}{n_{bound}} = e^{-\frac{\Delta\varepsilon}{kT}}$$

$$\Delta\varepsilon = E_{bond}$$

$$if \quad n_{broken} << n_{bound} \;\Rightarrow\; \frac{n_{broken}}{n_{bound}} \cong \frac{n_{broken}}{N}$$

The T7 DNA has about 40000 base pairs → has about 100 000 H-bonds → N= 100 000

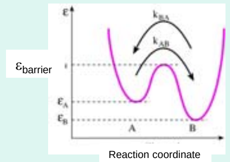
$$\boxed{\frac{n_{broken}}{n_{bound}} = e^{-\frac{\Delta\varepsilon}{kT}} = e^{-\frac{0.2}{0.026}} = 0.00046 \cong \frac{n_{broken}}{N} \qquad \Delta\varepsilon = E_{bond} = 0.2\,eV}$$

n_{broken} ~ 46/DNA
↑
time-average!

Significant number of secondary bonds are broken at body temperature → flexibility of macromolecular complexes → Possibility for ligand binding and chemical reactions

Boltzmann distribution - examples

2. Equilibrium rate of chemical reactions



Reaction : A ⟷ B

The ***k_{AB}*** and ***k_{BA}*** rates are proportional to the number of reactants which are higher in energy, reaching the top of the barrier

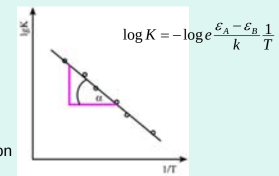
$$k_{AB} = const \times e^{-\frac{\varepsilon_{barrier} - \varepsilon_A}{kT}}$$

$$k_{BA} = const \times e^{-\frac{\varepsilon_{barrier} - \varepsilon_B}{kT}}$$

$$K = \frac{k_{BA}}{k_{AB}} = e^{-\frac{\varepsilon_A - \varepsilon_B}{kT}}$$

Experimental determination of the energy of activation

Arrhenius plot



3. Barometric formula

Density of air in the atmosphere decreases with the altitude (h) by the formula:

$$\boxed{\frac{\rho(h)}{\rho(0)} = e^{-\frac{mgh}{kT}}}$$

m average mass of particles in the air
g gravitational acceleration

End of the lecture