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Nuclear Fuel Cycle 2011

Lecture 2: Basic Nuclear Chemistry, Part 1

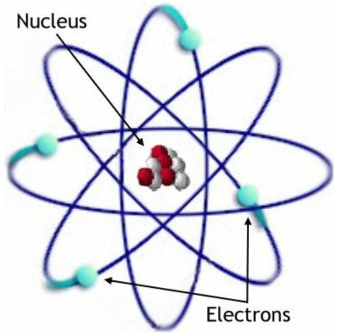
Home page of the course: KTH Social

https://www.kth.se/social/course/KD2430/

What is Nuclear Chemistry?

- Chemistry related to nuclear technology
- Chemistry of radionuclides
- Studies of chemical processes by using radionuclides as tracers: Radiochemistry
- Radiation induced chemical reactions: Radiation Chemistry

The Nucleus

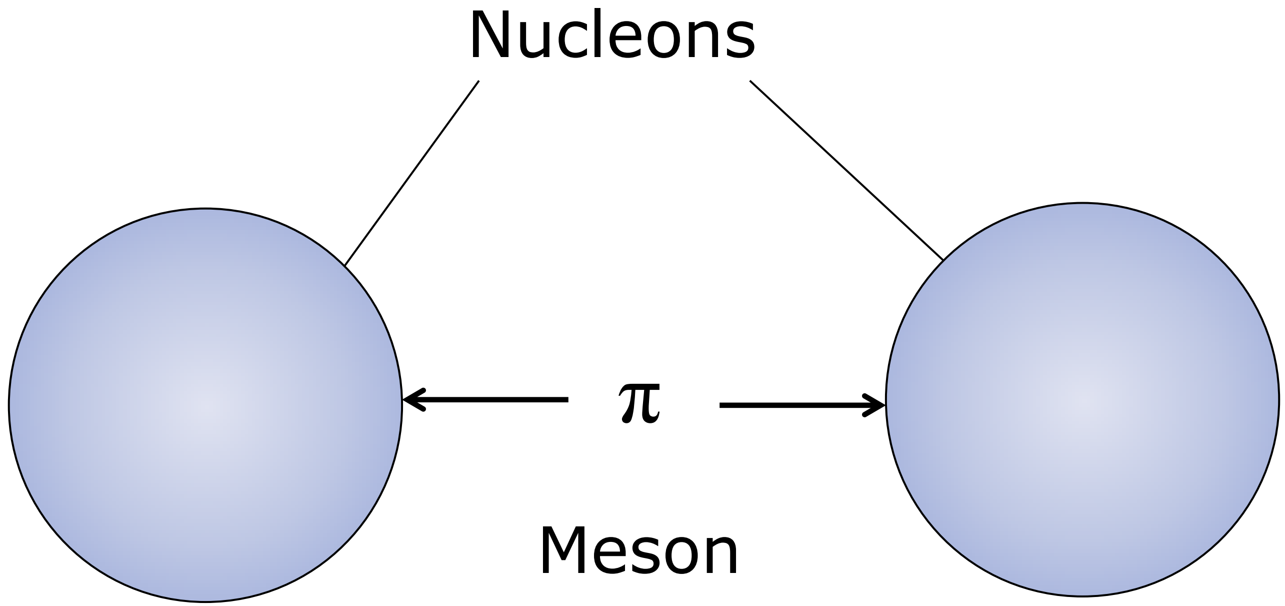


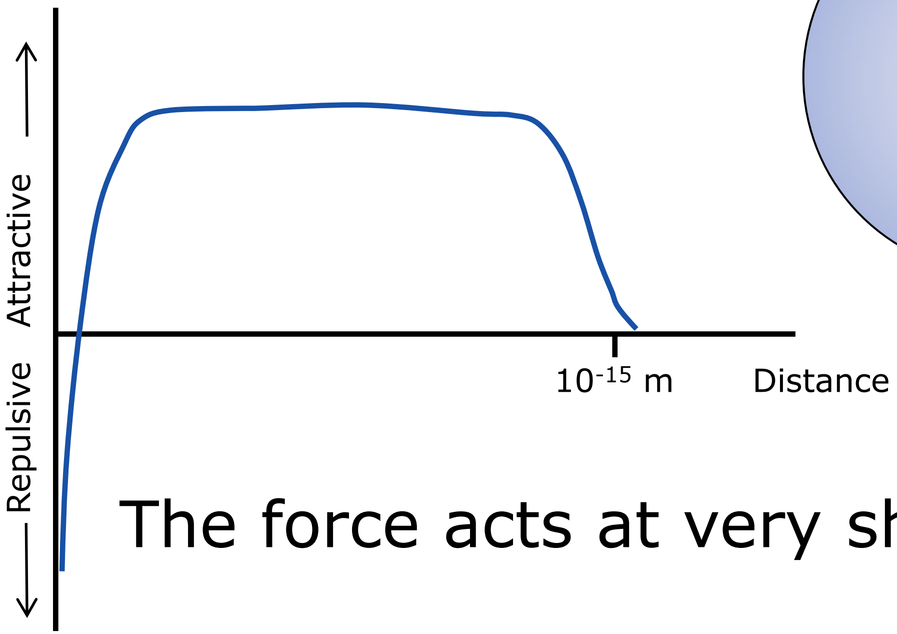
- Building blocks: Protons and neutrons
- Forces: Electromagnetic forces and the strong nuclear force

	Proton	**Neutron**
Mass	1.673×10^{-24} g	1.675×10^{-24} g
Charge	+1	0
Spin	s = ½	s = ½

The Strong Nuclear Force

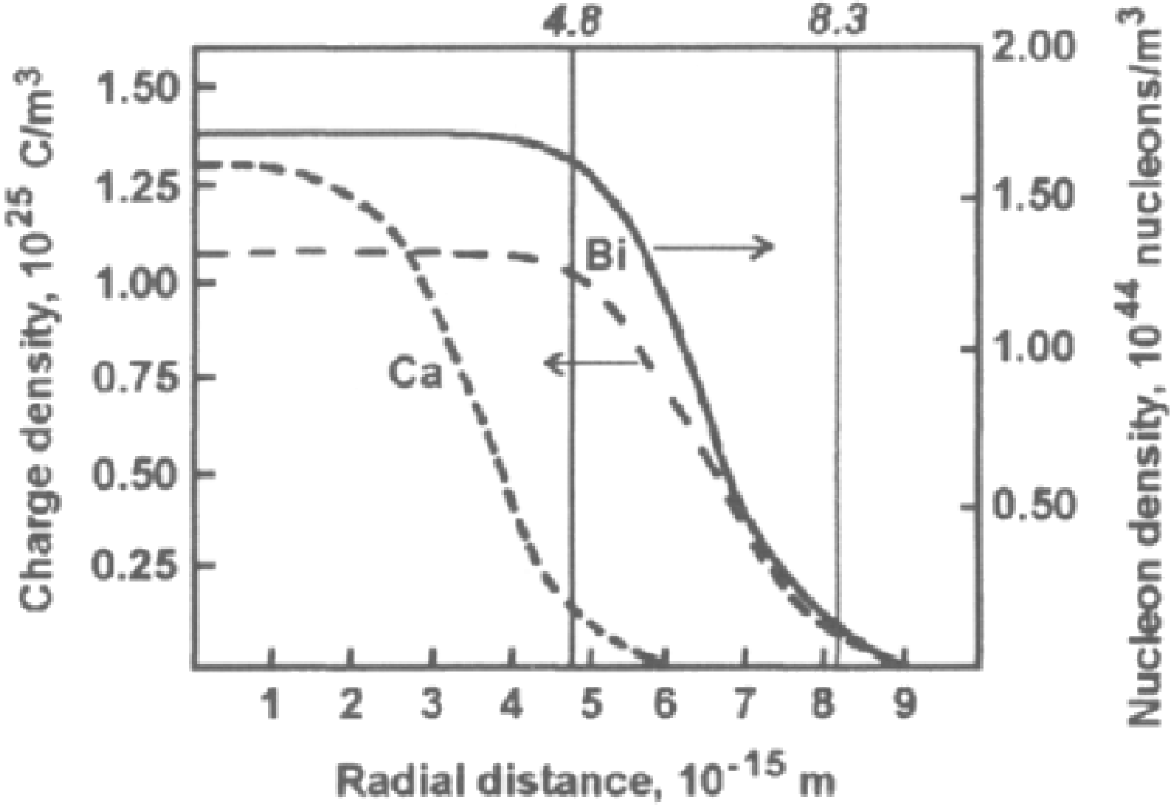
Exchange of mesons keep the nucleons together





The force acts at very short distances

Nuclear density and radius



Measured charge and nuclear density for ^{40}Ca and ^{209}Bi as a function of nuclear radius

Density: 0.2 nucleons/fm^3 => 10^{14} g/cm^3!

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The Nucleus

$$^{A}_{Z}R \qquad Z+N = A$$

Z = Number of protons

N = Number of neutrons

A = Mass number (number of nucleons)

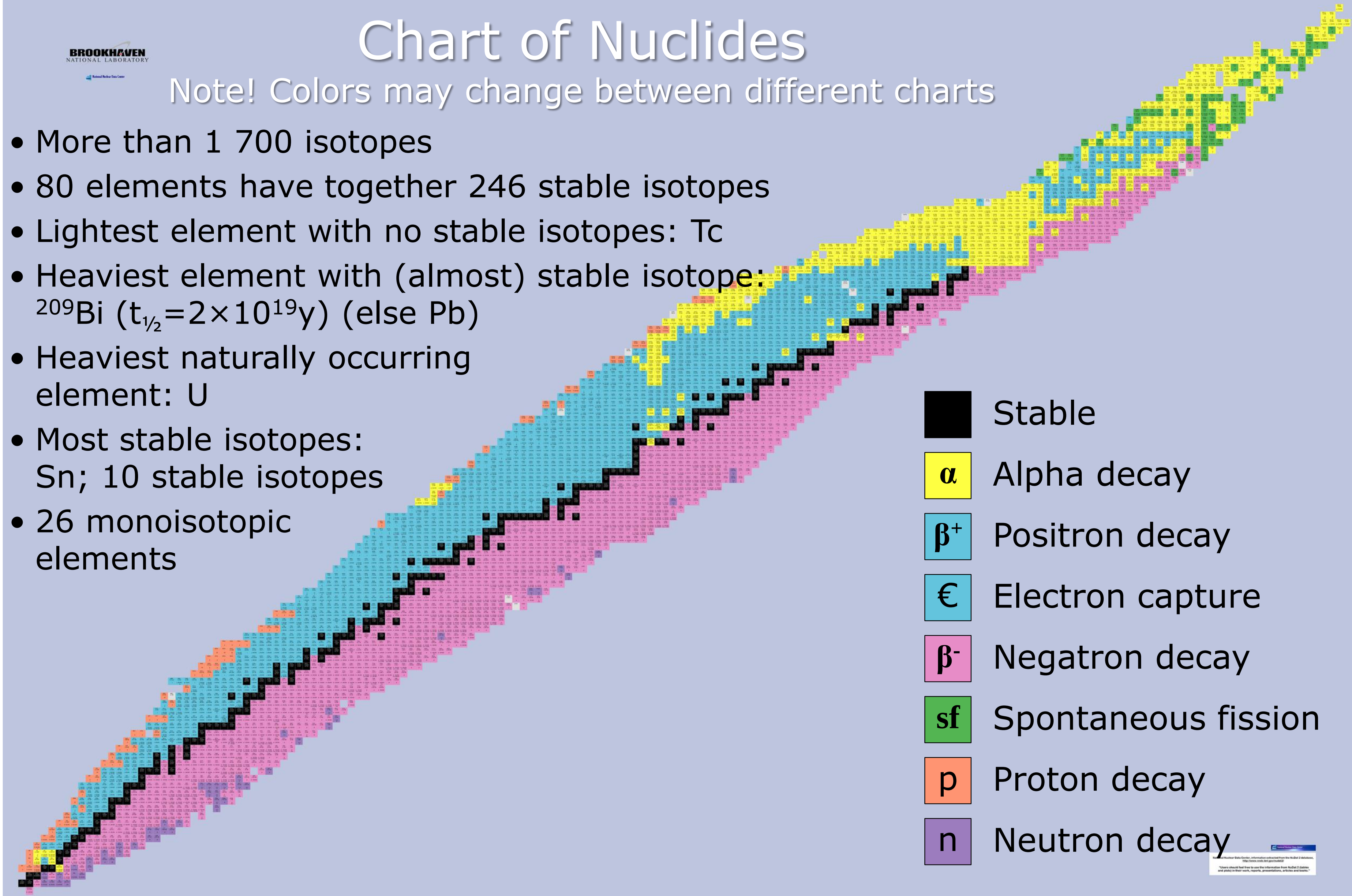
Nuclide	Specific nuclear species	Examples
Isotopes	Identical Z	$^{234}_{92}U$ $^{235}_{92}U$ $^{238}_{92}U$
Isotones	Identical N	$^{36}_{16}S$ $^{37}_{17}Cl$ $^{38}_{18}Ar$ $^{39}_{19}K$ $^{40}_{20}Ca$
Isobars	Identical A	$^{96}_{38}Sr$ $^{96}_{39}Y$ $^{96}_{40}Zr$
Isomers	Identical Z and A	$^{99m}_{43}Tc$ $^{99}_{43}Tc$

$$^{99m}_{43}Tc \xrightarrow{t_{1/2}=6.01h} {}^{99}_{43}Tc + \gamma$$

Chart of Nuclides

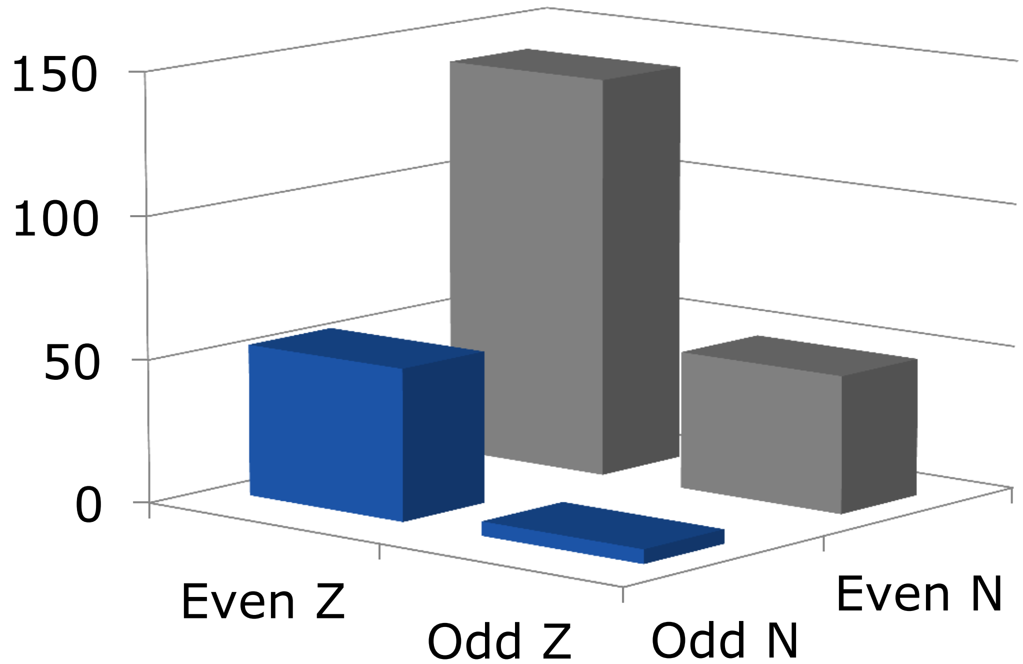
Note! Colors may change between different charts

- More than 1 700 isotopes
- 80 elements have together 246 stable isotopes
- Lightest element with no stable isotopes: Tc
- Heaviest element with (almost) stable isotope: ^{209}Bi ($t_{1/2}=2\times10^{19}$y) (else Pb)
- Heaviest naturally occurring element: U
- Most stable isotopes: Sn; 10 stable isotopes
- 26 monoisotopic elements



- Stable
- α Alpha decay
- β^+ Positron decay
- € Electron capture
- β^- Negatron decay
- sf Spontaneous fission
- p Proton decay
- n Neutron decay

Number of Nucleons on the Stability of the Nuclei



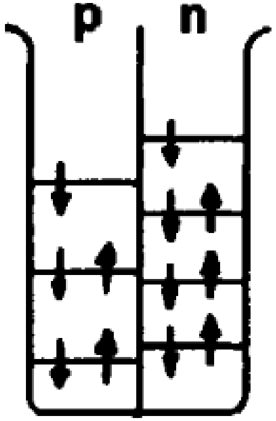
Magic numbers of protons or neutrons: 2, 8, 20, 82 and 126

$$^{135}_{54}Xe \ \left(\sigma_n = 2.6 \times 10^6 \text{ barns}\right) \ N = 81$$

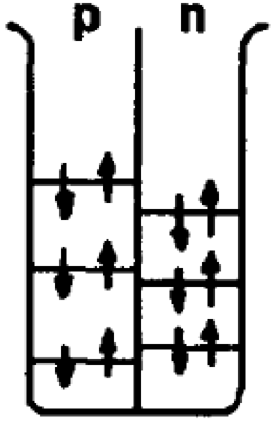
$$^{136}_{54}Xe \ \left(\sigma_n = 0.28 \times 10^6 \text{ barns}\right) \ N = 82$$

Nuclear Stability: Nucleon Orbitals

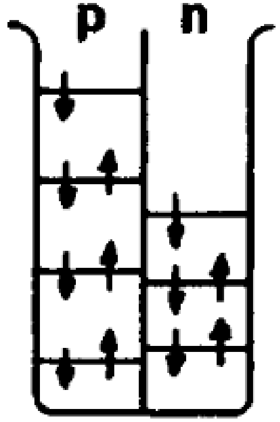
$^{12}_{5}B$ | $^{12}_{6}C$ | $^{12}_{7}N$



UNSTABLE



STABLE



UNSTABLE

$$^{12}_{5}B \longrightarrow {}^{12}_{6}C + e^-$$

$$(n \longrightarrow p + e^-)$$

$$^{12}_{7}N \longrightarrow {}^{12}_{6}C + e^+$$

$$(p \longrightarrow n + e^+)$$

Mass Defect (ΔM) and Mass Excess (δ_A)

$\Delta M_A = M_A - Z\, M_p - N\, M_n$

M_A = Mass of atom

M_H = Mass of Proton (hydrogen)

M_n = Mass of Neutron

Deuterium, ${}^{2}_{1}H$

$M_p + M_n = 1.007\,825 + 1.008\,665$
$= 2.016\,490$ u

$M_A = 2.014\,102$ u

=> $\Delta M_A = -0.002\,388$ u

All stable isotopes have negative mass defect, ΔM_A

Mass excess: $\delta_A = M_A - A$
(sometimes used in tables, no practical use)

M = atomic mass unit, measured in u.

Binding energy

$\Delta E = \Delta mc^2$ "Nuclear Heat of formation"

$\Delta m = M_A - (Z\ m_p + N\ m_n)$
$c = 3 \times 10^8$ m/s

Nucleus: 5-10 MeV / nucleon (5-10 $\times 10^{11}$ J/mol)

Covalent bond: 4.4 $\times 10^5$ J/mol

Isotope effects

Due to the difference in nucleons there are very small differences between two isotope's

- Freezing point
- Boiling point
- Density
- Heat of vaporization
- Viscosity
- Surface tension
- Optical emission spectra

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Isotope separation

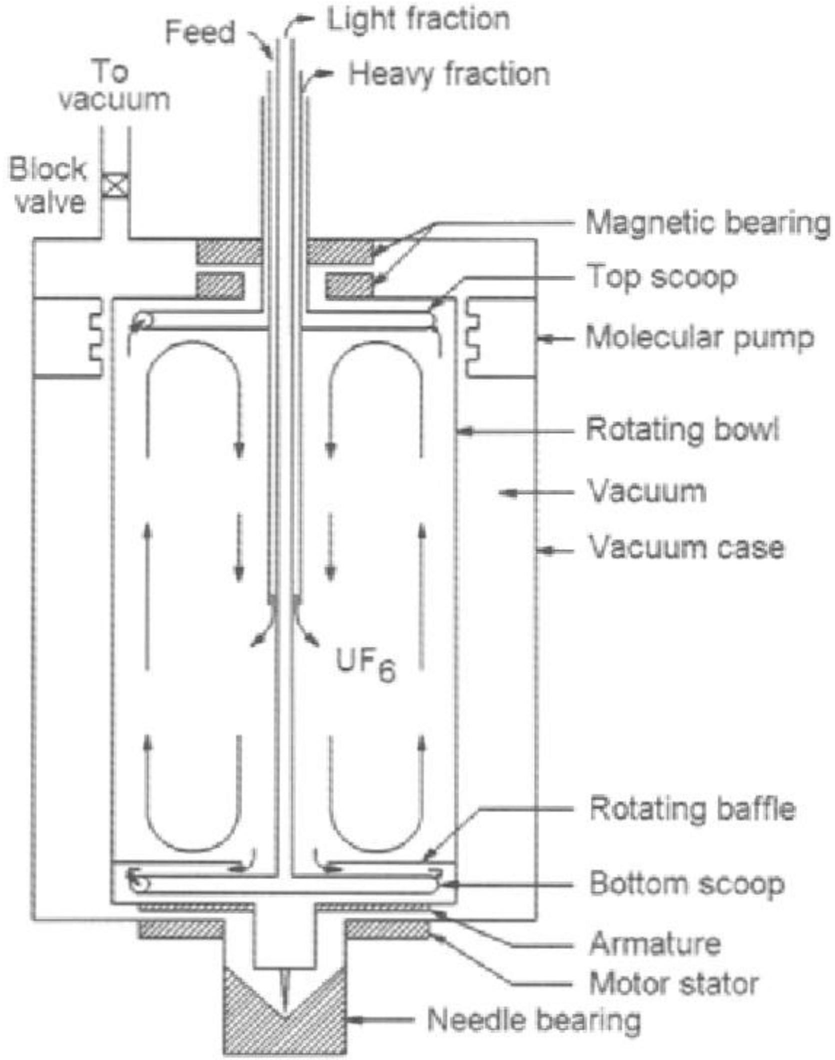
i. Equilibrium processes (light elements)
ii. Rate processes

- Multi-stage processes (for instance distillation)
- Chemical exchange
- Electrolysis
- Gaseous diffusion
- Electromagnetic separation
- Gas centrifugation

Gaseous diffusion

Lighter isotopes diffuse faster than heavy isotopes

$^{235}UF_6/^{238}UF_6$



Other methods of isotope separation

- Distillation
- Extraction
- Ion-exchange
- Photoionization
- Photoexcitation

Radioactive decay

- α-decay (He-nucleus)
- β-decay (electron/positron)
- γ-decay
- Unusual modes of decay (proton, neutron, heavy particles)
- Spontaneous fission

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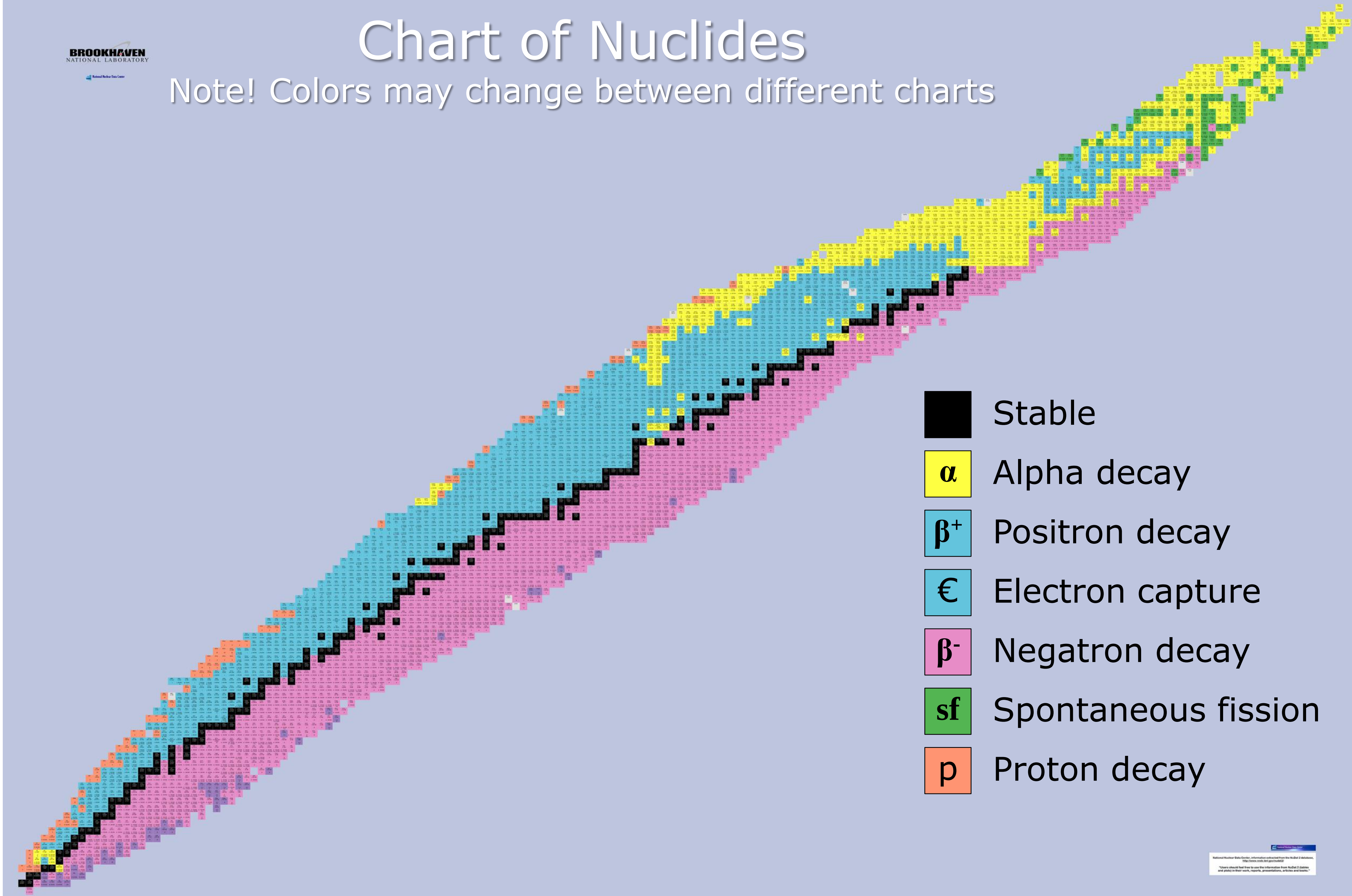
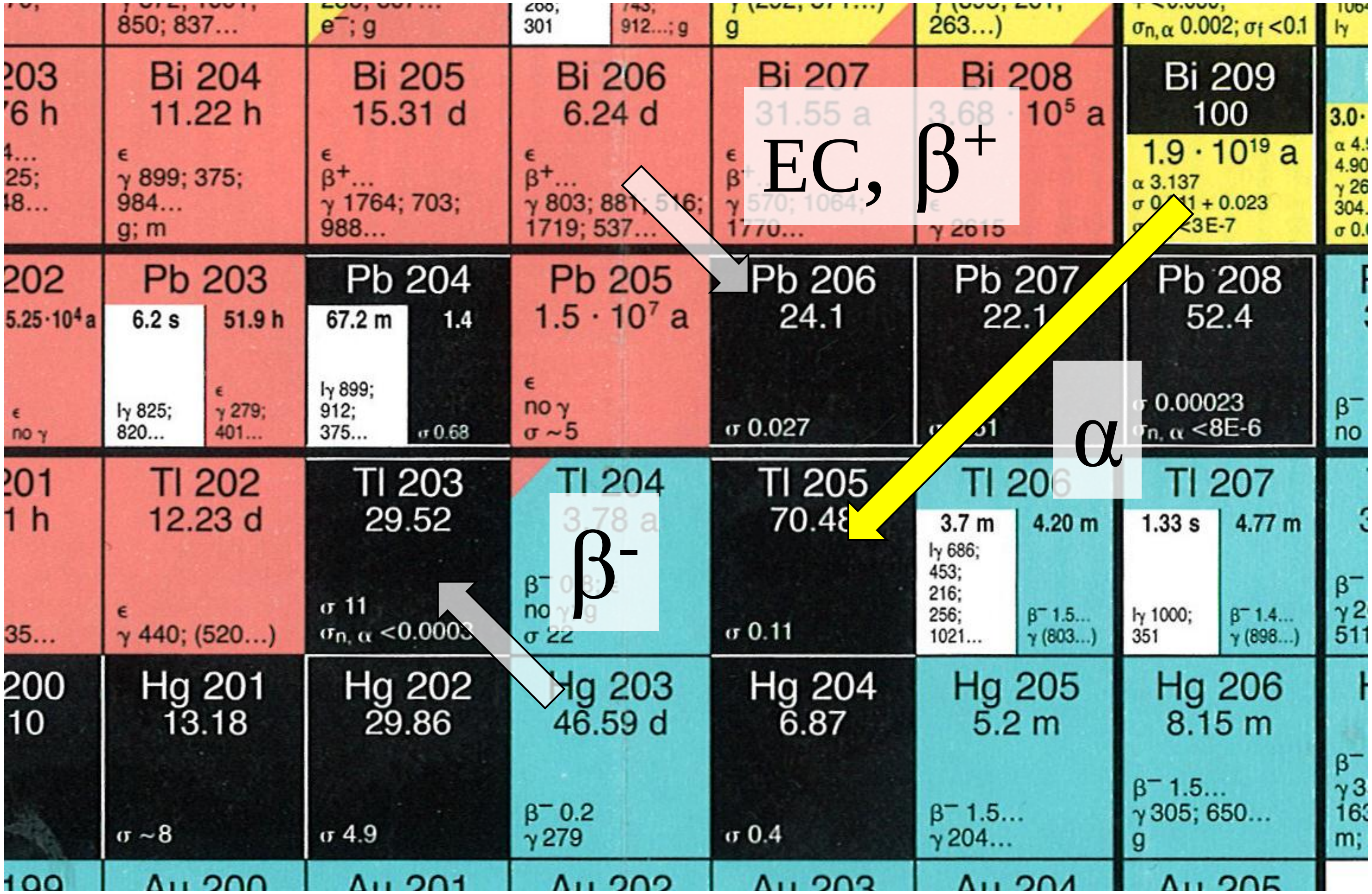
Chart of Nuclides

Note! Colors may change between different charts



Nuclide chart



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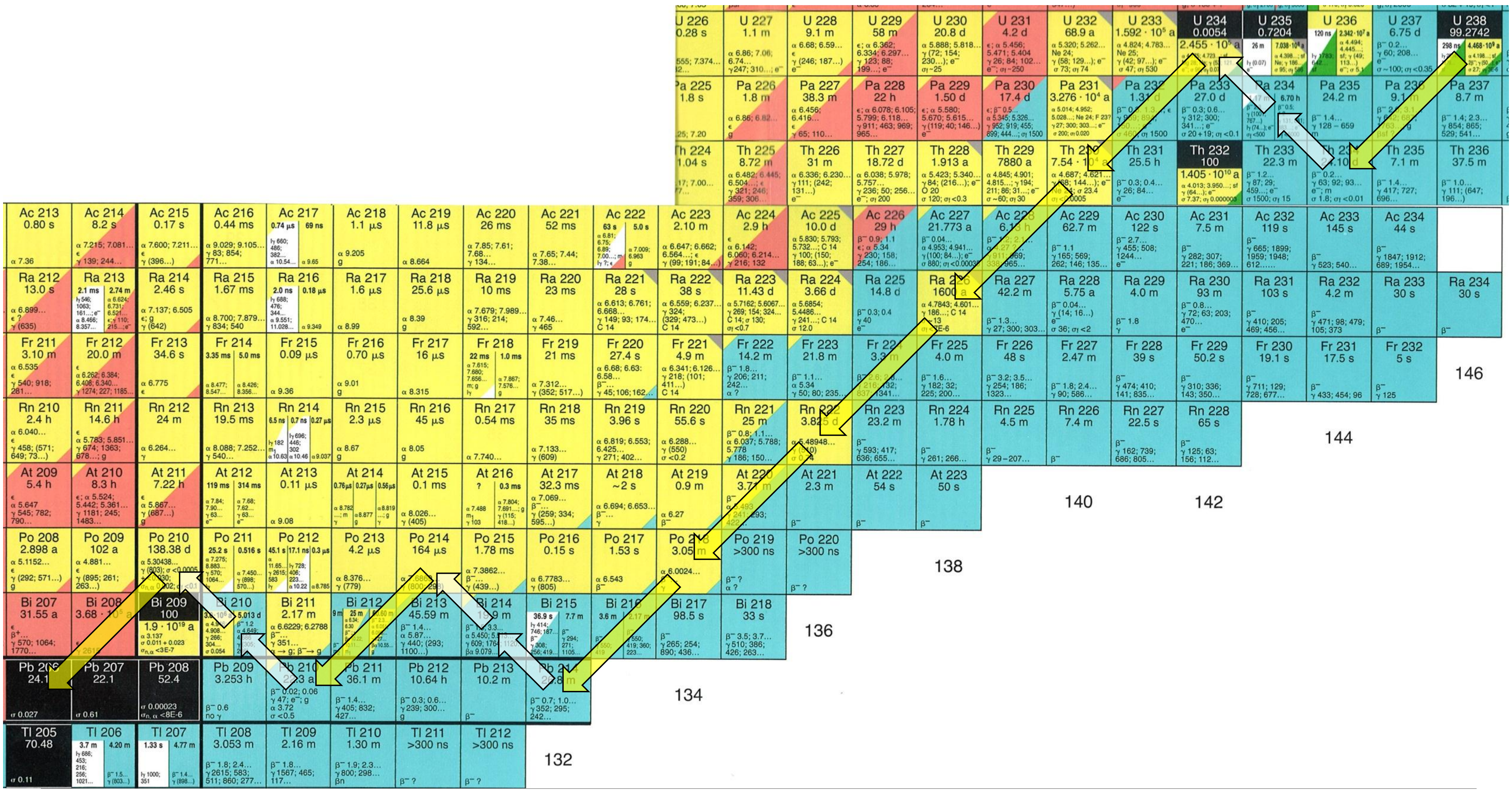
Decay chain of ^{238}U



Decay chain of ^{238}U

$^{238}U \rightarrow {}^{234}Th + \alpha$

$^{234}Th \rightarrow {}^{234}Pa + \beta^-$

$^{234}Pa \rightarrow {}^{234}U + \beta^-$

$^{234}U \rightarrow {}^{230}Th + \alpha$

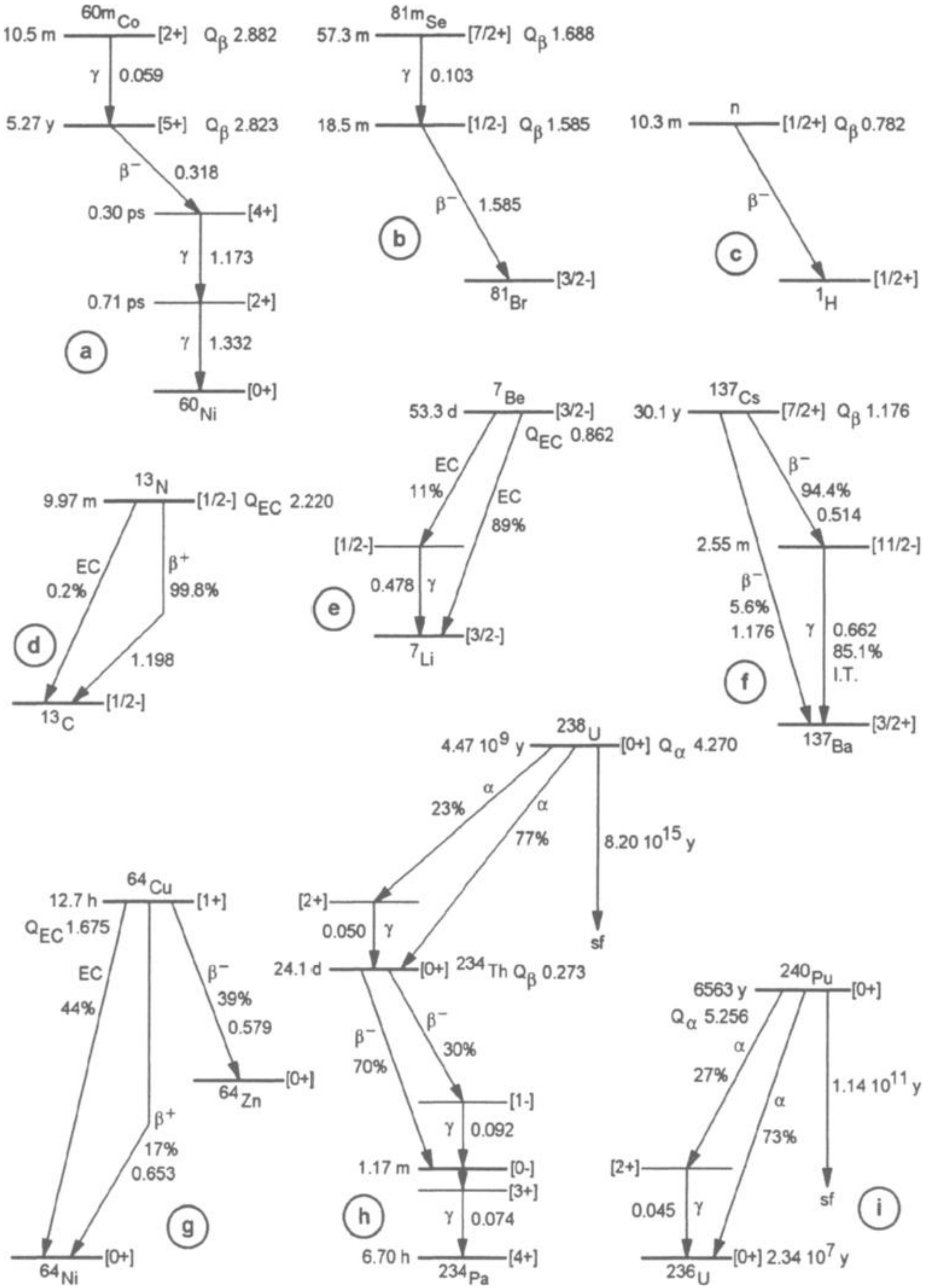
$^{230}Th \rightarrow {}^{226}Ra + \alpha$

...

Or simplified

$^{238}U(\alpha)\ {}^{234}Th(\beta^-)\ {}^{234}Pa(\beta^-)\ {}^{234}U(\alpha)\ {}^{230}Th(\alpha)\ {}^{226}Ra$...

Decay schemes



Conservation laws

Nuclear Reaction: $X_1 + X_2 \rightarrow X_3 + X_4$

Energy: $E_1 + E_2 = E_3 + E_4$

Linear momentum: $p=mv$

$p_1 + p_2 = p_3 + p_4$

Charge: $Z_1 + Z_2 = Z_3 + Z_4$

Mass number: $A_1 + A_2 = A_3 + A_4$

α-decay

$$^{A}_{Z}X \rightarrow \, ^{A-4}_{Z-2}Y + \, ^{4}_{2}He$$

$$^{238}U \rightarrow \, ^{234}Th + \, ^{4}He$$

Decay energy (Q-value)

$E = mc^2$

$1\ u = 1/6.022\times10^{23} = 1.66\times10^{-24}$ g

$c^2 = 8.99\times10^{16}\ m^2/s^2$

$1\ J = 6.24\times10^{12}$ MeV

$E = 1.66\times10^{-24} * 8.99\times10^{16} * 6.24\times10^{12} = 931.5$ MeV/u

Q(MeV) = -931.5 ΔM (u)

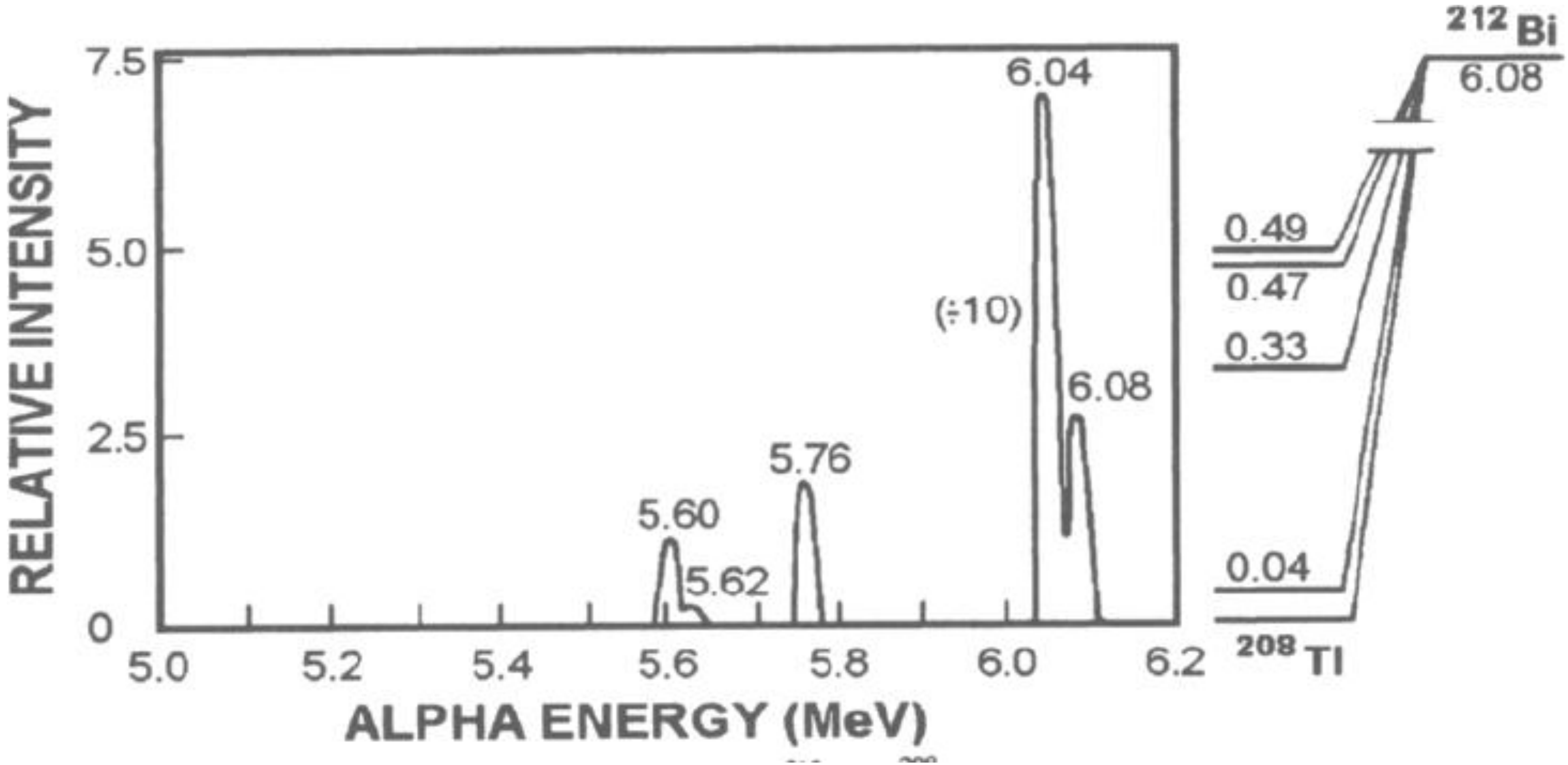
$Q_\alpha = -931.5\ (M_{Z-2} + M_{He} - M_Z)$

$Q_\alpha > 0$ if $(M_{Z-2} + M_{He} - M_Z) < 0$

$Q_\alpha > 0$ => Spontaneous decay

For α-particles the Q-value is 2–10 MeV

Alpha spectrum



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β-decay

$${}^{A}_{Z}X \rightarrow {}^{A}_{Z+1}Y + \beta^{-}$$

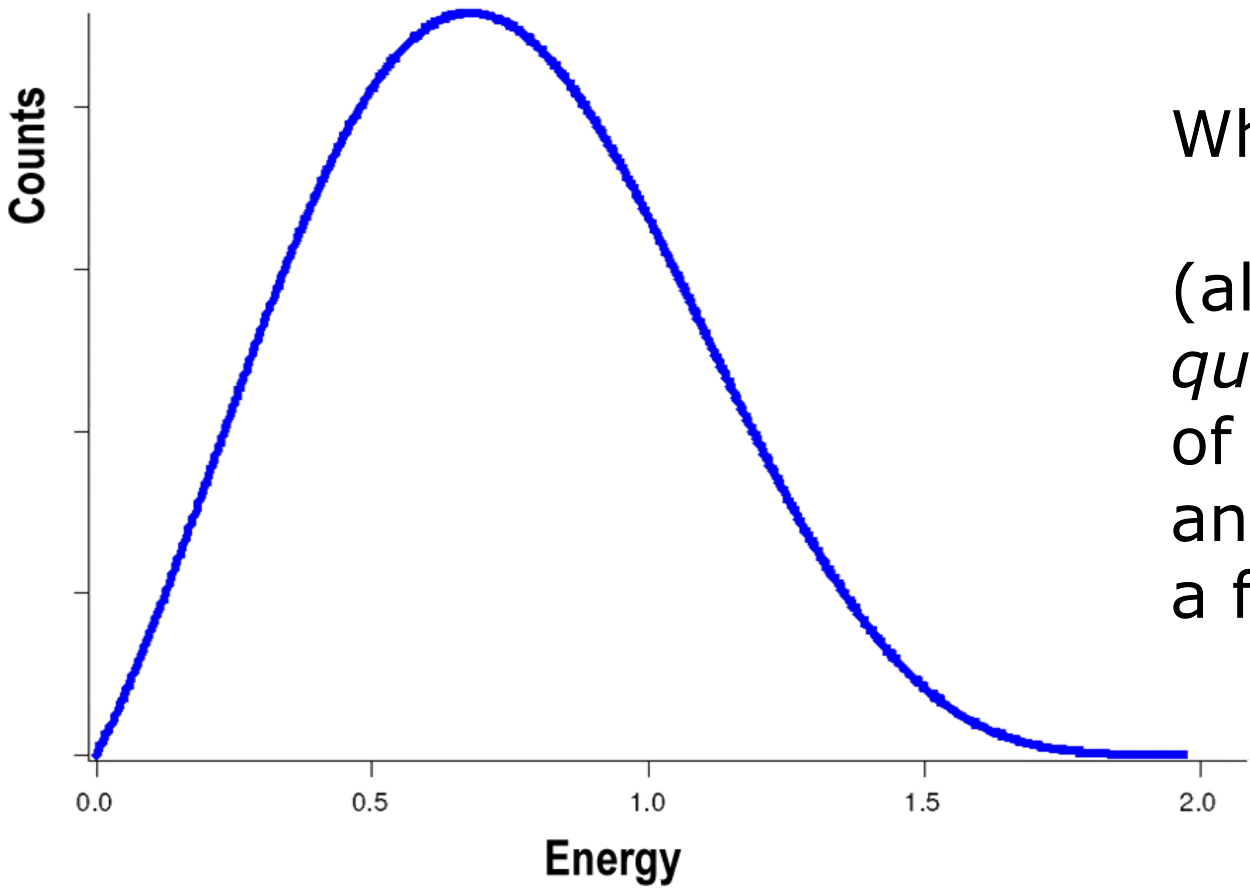
A negatron (electron) is emitted
A proton in the nucleus is 'coverted' to a neutron

$${}^{A}_{Z}X \rightarrow {}^{A}_{Z-1}Y + \beta^{+}$$

A positron (anti-partivle to the electron) is emitted.
A neutron in the nucleus is 'converted' to a proton

β-decay

$$^{137}Cs \rightarrow {}^{137m}Ba + \beta^-$$



Why not one peak?

(also the *nuclear spin quantum number* of the reaction is not an integer, which is a forbidden transition)

β-decay continued

$\Rightarrow$ Another particle is emitted: a neutrino (ν)

The neutrino has no charge and very small or no mass and does not interact readily with matter

$$^{137}Cs \rightarrow {}^{137m}Ba + \beta^- + \bar{\nu}$$

$\bar{\nu}$ is an anti-neutrino, emitted in a β^--decay

ν is a neutrino, emitted in a β^+-decay

Energy of β⁻ decay

$$^{A}_{Z}X \rightarrow {}^{A}_{Z+1}Y + \beta^{-} + \bar{\nu}$$

The formed Y has Z orbit electrons and must capture one electron from the surroundings.

=> The mass of the β^{-}-particle needs not to be included when calculating the energy of the decay.

$$Q_{\beta-} = -931.513\ (M_{Z+1} - M_{Z})$$

Example: $n \rightarrow H + \beta^{-}$

$$Q_{\beta-} = -931.513(1.007825-1.008665) = 0,782\ \text{MeV}$$

Energy of β^+ decay

$$^{A}_{Z}X \rightarrow {}^{A}_{Z-1}Y^{-} + \beta^{+} + \nu \rightarrow {}^{A}_{Z-1}Y + e^{-} + \beta^{+} + \nu$$

The formed Y has now one extra orbit electron which it must loose.

=> Both emitting a β^+-particle and loosing an electron must be included when calculating the energy of the decay.

$$Q_{\beta-} = -931.513\ (M_{Z-1} + 2\ M_e - M_Z)$$

Example: $^{13}_{7}N \rightarrow {}^{13}_{6}C + \beta^{+}$

$$Q_{\beta-} = -931.513(13.003355 - 13.005739) + 2 * 0.511) = 1,2\ MeV$$

Electron capture

$$^{A}_{Z}X \xrightarrow{EC} {}^{A}_{Z-1}Y + \nu$$

An inner shell electron is captured by the nucleus.

Energy similar to β^- decay.

$$Q_{\beta-} = -931.513\ (M_{Z-1} - M_Z)$$

γ-emisson

Most α and β-decays do not go all the way to the daughter's ground state.

The remaining energy is released as γ-rays.

Isomeric transition

When the meta-stable state is more long-lived

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Spontaneous fission

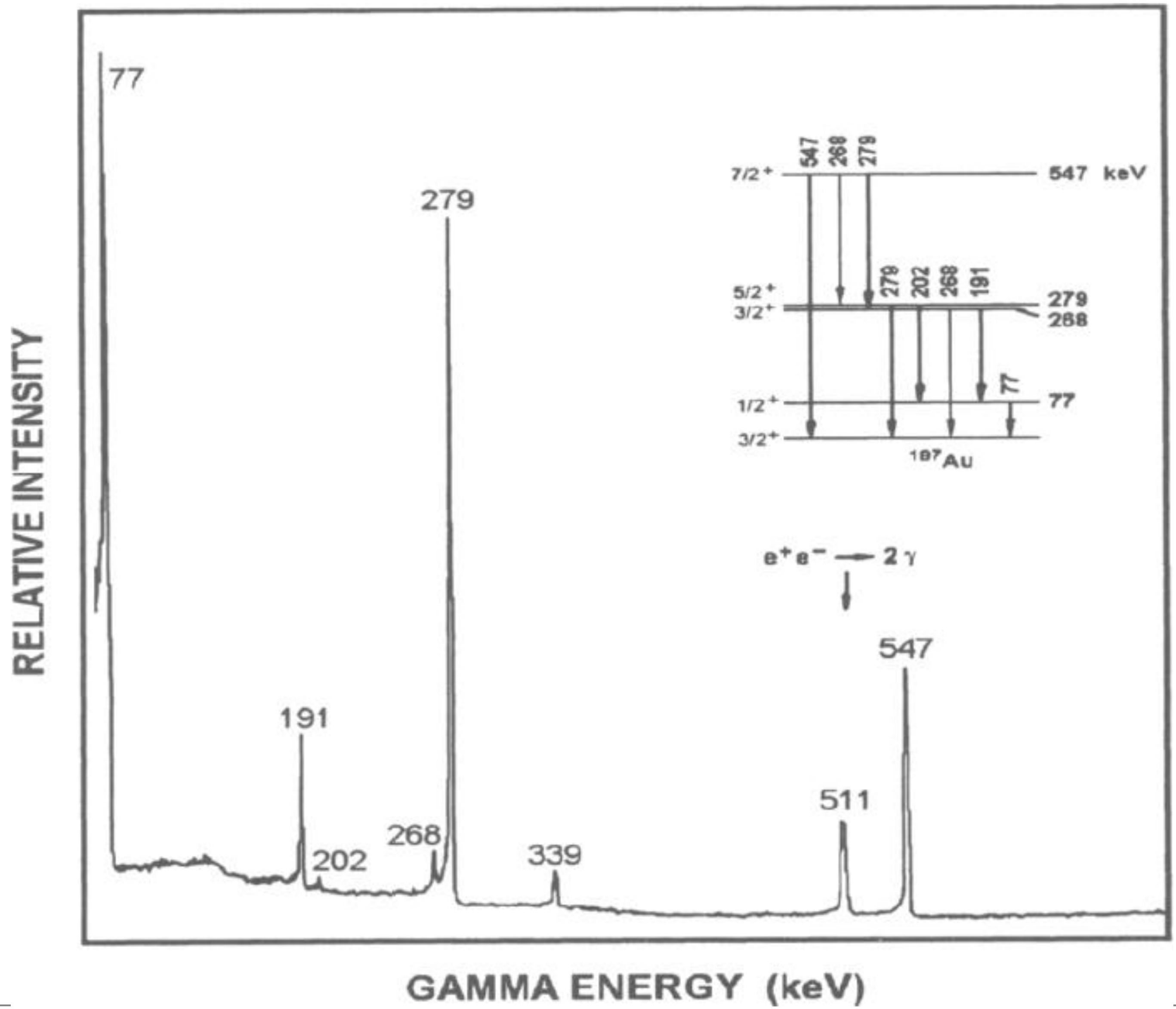
Some heavy radionuclides are so unstable that they undergo spontaneous fission

Rare modes of decay

Proton emission

Neutron emission

Gamma spectrum



Radioactive decay

$$A = -\frac{dN}{dt} = \lambda N$$

$$-\frac{dN}{N} = \lambda dt$$

$$-\int_{N_0}^{N} \frac{1}{N} dN = \int_{0}^{t} \lambda dt \Rightarrow \ln N - \ln N_0 = -\lambda t$$

$$N = N_0 e^{-\lambda t}$$

Half-life

$$-\int_{N_0}^{N} \frac{1}{N} dN = \int_0^t \lambda dt \Rightarrow \ln N - \ln N_0 = -\lambda t$$

$$N = \frac{N_0}{2}$$

$$t_{½} = \frac{\ln N_0 - \ln\left(\frac{N_0}{2}\right)}{\lambda} = \frac{\ln 2}{\lambda}$$

Units

SI unit:

1 Becquerel (Bq) = 1 decay / s

Older unit:

1 Curie (Ci) = 3.7×10^{10} Bq

(1 Ci is approximately the actvity of 1 gram ^{226}Ra)