

Correction for Test I – Duration : 1h

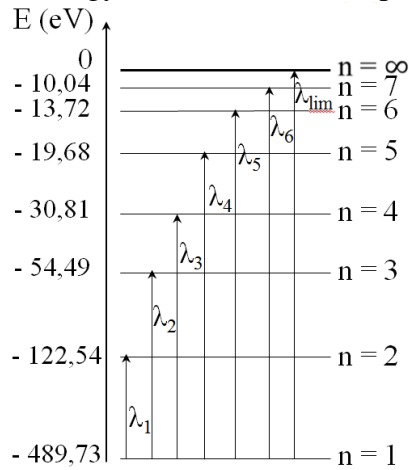
I. Atomic model (6 points)

- 1) n : main quantum number, characterizes the size of the orbital or numbers the electronic shell ; n being a positive integer (> 0)
 ℓ : secondary quantum number, characterizes the shape of the orbital or numbers the sub-shell;
 $0 \leq \ell \leq n-1$
 m_ℓ : magnetic quantum number or orbital, characterizes the orientation of the orbitals in space, or the quantum boxes, $-\ell \leq m_\ell \leq +\ell$
 m_s : spin quantum number, characterizes the spin and the quantification of the kinetic moment of the electron, $m_s = \pm 1/2$
- 2) a) **FALSE** : if $\ell = 1$, the electron is in a p sub-shell (not d)
 b) **FALSE** : if $n = 4$, the electron is in the N shell (not O, which $n = 5$)
 c) **FALSE** : for a d electron, as $\ell = 2$, m_ℓ can be equal to -2, -1, 0, 1, 2 (but not 3)
 d) **FALSE**, for a (3)d subshell : $\ell = 2$; $m_\ell = -2, -1, 0, 1, 2$; 5 quantum boxes, each occupied at best by 2 electrons : can be occupied by maximum 10 electrons (and not 6)
 e) **FALSE** : $n = 3$, $\ell = 0, 1, 2$ that correspond respectively to the s, p and d orbitals : no f exists. For an electron to be in a f-subshell ($\ell = 3$), n has to be at least equal to 4.
 f) **TRUE**
 g) **TRUE**

II. Spectroscopy of an hydrogen-like system (14 points)

- 1) In an **absorption spectrum**, the rays that are observed correspond to transitions from $n = 1$ to **upper levels**.
 As wavelength and energy varies in an opposite way:
 λ_I owns the highest wavelength, thus corresponds to the transition with the smallest energy, thus involving levels that are the closest to each other : starting from $n = 1$, it corresponds to the transition from $n = 1$ to $n = 2$
 λ_{II} owns the 2nd highest wavelength, thus corresponds to the transition with the 2nd smallest energy, thus involving the second closest level to $n = 1$: it corresponds then to the transition from $n = 1$ to $n = 3$
 etc....
 λ_{∞} owns the smallest wavelength, thus corresponds to the transition with the highest energy, involving the furthest level to level $n = 1$: it corresponds then to the transition from $n = 1$ to $n = \infty$
- λ_I : transition $n = 1$ to $n = 2$, $E_2 - E_1 = \frac{h \times c}{e \times \lambda_I} = 367.19 \text{ eV}$; λ_{II} : transition $n = 1$ to $n = 3$, $E_3 - E_1 = \frac{h \times c}{e \times \lambda_{II}} = 435.24 \text{ eV}$
 λ_{III} : transition $n = 1$ to $n = 4$, $E_4 - E_1 = \frac{h \times c}{e \times \lambda_{III}} = 458.92 \text{ eV}$; λ_{IV} : transition $n = 1$ to $n = 5$, $E_5 - E_1 = \frac{h \times c}{e \times \lambda_{IV}} = 470.05 \text{ eV}$
 λ_V : transition $n = 1$ to $n = 6$, $E_6 - E_1 = \frac{h \times c}{e \times \lambda_V} = 476.01 \text{ eV}$; λ_{VI} : transition $n = 1$ to $n = 7$, $E_7 - E_1 = \frac{h \times c}{e \times \lambda_{VI}} = 479.69 \text{ eV}$
 λ_{∞} : transition $n = 1$ to $n = \infty$, $E_\infty - E_1 = \frac{h \times c}{e \times \lambda_{\infty}} = 489.73 \text{ eV}$
- Careful with the precision that was required !!!!*
- 2) From $E_\infty - E_1 = \frac{h \times c}{e \times \lambda_{\infty}} = 489.73 \text{ eV}$, and as $E_\infty = 0$ and values are set as negative: $E_1 = - 489.73 \text{ eV}$
- 3) From question 1, we computed $E_n - E_1$. From question 2, we have E_1
 Thus $E_2 = (E_2 - E_1) + E_1 = \frac{h \times c}{e \times \lambda_I} + E_1$
 $E_2 = - 122.54 \text{ eV}$ $E_3 = - 54.49 \text{ eV}$ $E_4 = - 30.81 \text{ eV}$
 $E_5 = - 19.68 \text{ eV}$ $E_6 = - 13.72 \text{ eV}$ $E_7 = - 10.04 \text{ eV}$

Resulting Grotrian's diagram with the energy levels and the absorption rays (each being identified!!!)



4) Using Ritz-Balmer equation and the ionization energy that corresponds to the transition from $n = 1 \rightarrow n \infty$: $Z = \sqrt{\frac{E_i}{h \times c \times R_X}} = 6$: thus the hydrogen-like ion is ${}_6X^{5+}$

5) $E_i = -E_1 \times N_A = 4.724 \cdot 10^4 \text{ kJ} \cdot \text{mol}^{-1}$ (careful with the number of significant digits!!!)

6) a) Ray $\lambda_V = 26.05 \text{ \AA}$ corresponds to the transition from $n = 1$ to $n = 6$.
As we want to observe this transition, we need to provide at least the energy that corresponds to this transition: this defines the minimum energy (if you provide less than $E_{1 \rightarrow 6}$, absorption will not occur !!!).

Because we only want the given transition, we need to provide strictly less energy than the one required to promote the electron to $n = 7$: this defines the maximum energy.

Thus : $E_{1 \rightarrow 6} \leq E < E_{1 \rightarrow 7}$

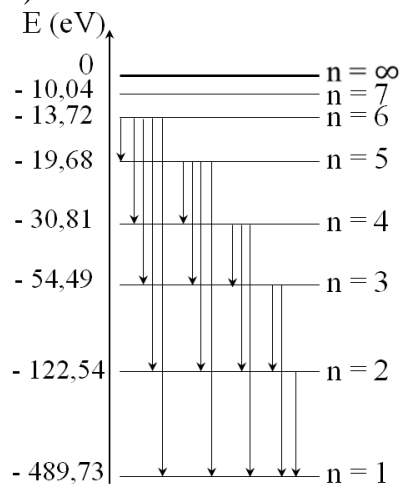
As energy and frequencies are proportional to each other, we have : $\nu_{1 \rightarrow 6} \leq \nu < \nu_{1 \rightarrow 7}$

$$\nu_{1 \rightarrow 6} = \frac{E_6 - E_1}{h} = 1.151 \cdot 10^{17} \text{ Hz}$$

$$\nu_{1 \rightarrow 7} = \frac{E_7 - E_1}{h} = 1.159 \cdot 10^{17} \text{ Hz}$$

(careful with the number of significant digits!!!)

b) After excitation to level $n = 6$, we may observe 15 rays in the corresponding emission spectrum



c) As the ionization energy for hydrogen is 13.60 eV, the two radiations that own a lower energy are:
i. Transitions from $n = 6$ down to $n = 5$ ($E_{6 \rightarrow 5} = 5.96 \text{ eV}$) and from $n = 5$ down to $n = 4$ ($E_{5 \rightarrow 4} = 11.13 \text{ eV}$)
ii. The corresponding wavelengths are then $\lambda_{6 \rightarrow 5} = 207 \text{ nm}$ and $\lambda_{6 \rightarrow 5} = 112 \text{ nm}$.
iii. They belong to the UV domain

7) $E_T \text{ (eV)} = E_i \text{ (eV)} + E_c \text{ (eV)} = E_i \text{ (eV)} + \frac{1}{2} \frac{mv^2}{e} = 489.73 + 2.84 = 492.57 \text{ eV}$
(careful with the precision that was required!!!)