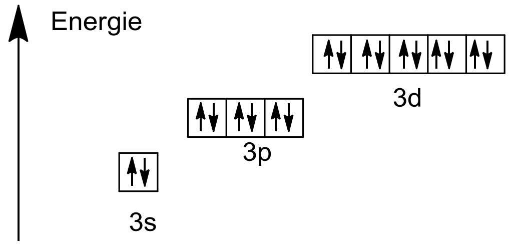
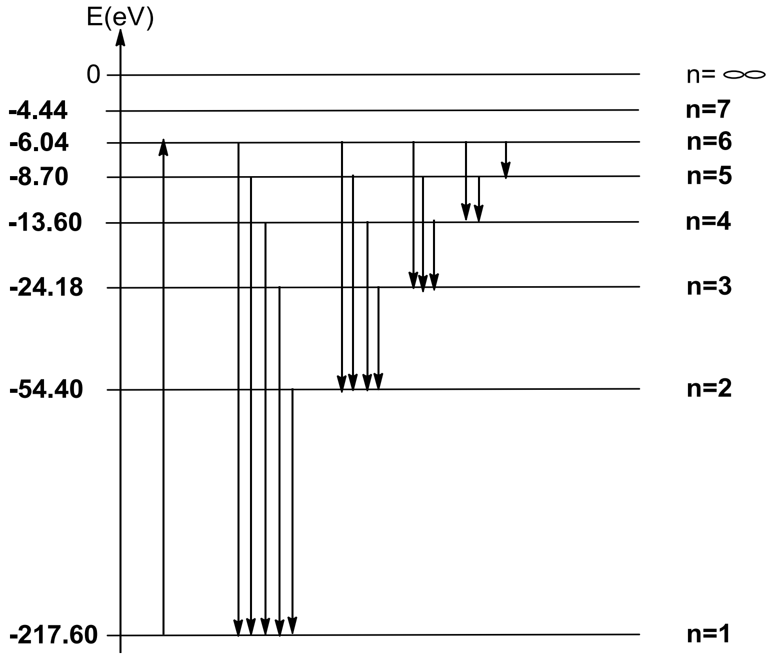
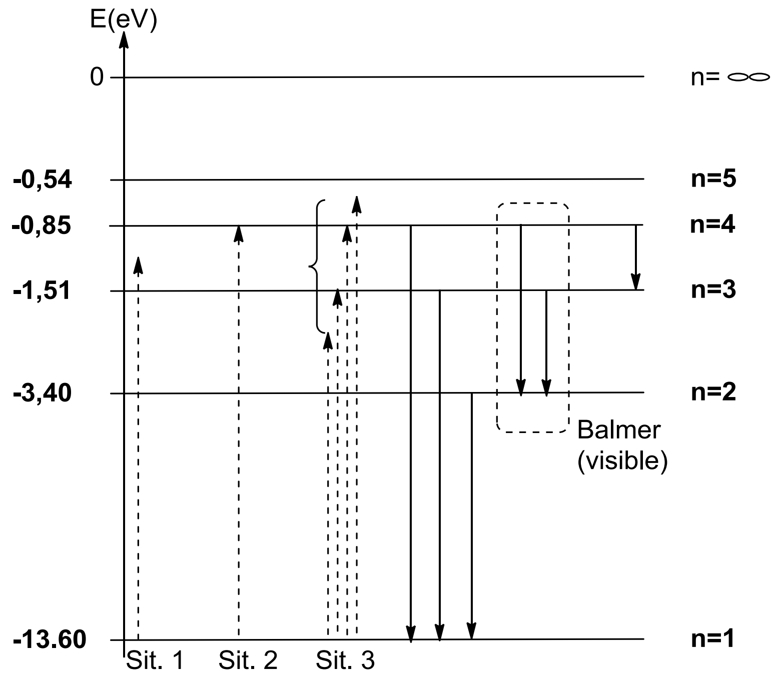
CHEMISTRY Test n°1 18/10/2019 – Some answers and comments

	Problem 1 : Quantum numbers and electronic configuration	Some comments
a)	n : integer values ≥ 1 or 1, 2, 3, 4…n l : integers values 0 ≤l ≤ n-1 or 0, 1, 2, 3, 4…(n-1) m :integer values -l ≤ m ≤ +l or -l, -l+1…. 0…., l-1, l s : ± 1/2	Lack of precision: n, l and m are **integers;** while s is not. For example, stating that 0 ≤l ≤ n-1 is not enough
b)	For n = 3, l = 0 (2 electrons) or 1 (6) or 2 (10) = total 18 electrons	Generally well understood
c)		The question was to represent the levels on **an energy scale,** not only to represent the quantum boxes
d)	n=3 l=0 m=0 s=± ½ n=3 l=1 m=-1, 0, +1 s=± ½ n=3 l=2 m=-2,-1,0,+1,+2 s=± ½	Stating that l = 0, 1 or 2 and m = -2, -1, 0, 1, 2 etc **is WRONG** It was expected to have the set of possible values for m depending on the corresponding value of l (see on the left)
e)	n=5 l=3 m=-3,-2,-1,0,+1,+2,+3 s=± ½	
f)	**Pauli:** An atom can not have 2 electrons with the same set of values for the quantum numbers n, l, m and s **Hund:** pairing electrons with opposite spins cost energy : all orbitals of a subshell must be each occupied by a single electron before any of them being occupied by two paired electrons. **Klechkowski** : subshells are filled according to increasing values of (n+l), and according to values of n for two identical values of (n+l)	Rules are in general known, even if the names are sometimes mixed up (but no penalty)
g)	$_{7}N$: $1s^2\ 2s^2\ 2p^3$ $_{31}Ga$: $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 3d^{10}\ 4s^2\ 4p^1$	

	${}_{47}Ag$: $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 3d^{10}\ 4s^2\ 4p^6\ 4d^{10}\ 5s^1$ ${}_{52}Te$: $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 3d^{10}\ 4s^2\ 4p^6\ 4d^{10}\ 5s^2\ 5p^4$	
h)	Number of single electrons: 3 Ga: 1 Ag: 1 Te: 2	Representation of quantum boxes and split of electrons may help to answer this question that concerned single electrons. Some confusion with valence electrons.

	Problem 2 : Study of a hydrogen-like ion	**Some comments**
a)	The energy required to extract the electron from the ion	For an hydrogen-like system, before ionization it was already an ion by definition: stating that the consequence is to end up with an ion is wrong
b)	Transition level 1→∞ Smallest λ : Serie's limit	In the Bohr model, the transition is from a level (not a *subshell*, not an *orbital*) and involves the unique electron (not *an* electron)
c)	$\frac{1}{\lambda} = R_X Z^2 \left(\frac{1}{n^2} - \frac{1}{n'^2}\right)$ et $E = \frac{hc}{\lambda}$ gives $\Delta E_{limit} = \lvert E_1 - E_\infty \rvert = \frac{hC}{\lambda} = \mathrm{hC}R_X Z^2 \left(\frac{1}{1^2} - \frac{1}{\infty^2}\right) = \mathrm{hC}R_X\, Z^2 = -E_1$ with $E_n = 0\ and\ E_1 < 0$)	Some errors on manipulation of equation. Remember that ΔE is positive, while E_1 or E_n is negative by convention By the way, the relation $E = \frac{hc}{\lambda}$ is not de Broglie's equation as it found in some copies!
d)	$E_{ionization} = -E_1 = E(ev) * e * N_A * 10^{-3} = 20\,990\ kJ.mol^{-1}$	Conversion eV/J/KJ has led to some mathematical errors
e)	$Z = \sqrt{\frac{-E_1(J)}{hCR_X}}$ Z=4 ${}_4Be^{3+}$	Literal expressions were often given, but some mathematical errors were found. Indeed, if *c* is used in (m/s) then R_X should be expressed in (m^{-1}); if you keep R_X in (cm^{-1}), then *c* should be expressed in (cm/s).
f)	$\lvert E_n - E_\infty \rvert = \frac{hC}{\lambda} = \mathrm{hC}R_X Z^2 \left(\frac{1}{n^2} - \frac{1}{\infty^2}\right) = \frac{\mathrm{hC}R_X\, Z^2}{n^2}$ $\frac{E_1}{n^2} = E_n$ (with $E_n < 0$)	Many of you do not know how to find E_n from Ritz-Balmer. Some confusions between E_1 and $E_{ionization}$ $E_n = \frac{E_1}{n^2} = -\frac{E_{ionization}}{n^2}$ E_1 is the energy level of the hydrogen-like system and not the one for hydrogen : so $E_n \neq \frac{Z^2 E_1}{n^2}$ as found in some copies

g)	E_1=-217.60 eV ; E_2=-54.40 eV ; E_3=-24.18 eV ; E_4=-13.60 eV ; E_5=-8.70 eV ; E_6=-6.04 eV ; E_7=-4.44 eV	Many of you know that $E_n = \frac{E_1}{n^2}$ and where then able to answer this question Careful with the expected precision (to within 0.01 eV)
h)		This diagrame requires : - A legend (E(eV) - The origin of the energy scale for n →∞ - Each energy level (up to n = 7), with the associated energy (value or identification E_1…)
i)	Absorption up to n = 6 Then a total of 15 rays Represented on the diagram	

	Problem 3 : Hydrogen spectroscopy	Some Comments
a)		This diagram requires : - A legend (E(eV) - The origin of the energy scale for n $\rightarrow\infty$ - Each energy level (up to n = 5), with the associated energy (value or identification E_1…)
	<u>Situation 1 :</u> E_{ex}=12400/1000=12.40eV= $\lvert E_{arrival} - E_1 \rvert$ such that $E_{arrival}$ = - 1.20 eV This does not correspond to the energy of a level for hydrogen: because the energy is quantified, there is no excitation at all for hydrogen. No absorption thus no emission : the corresponding spectrum is then spectrum E	Some confusion here : - Many of you have used the value of the *incoming radiation* and concluded that it does not belong to the visible range: the reasoning is WRONG. The value of the wavelength given in the subject is the one of the incoming radiation (that lead to excitation or not) and not the one of the emitted photon. Indeed, the detector records the emitted lines.

	<u>Situation 2 :</u> E_{ex}=12400/972.5=12.75 eV = $\lvert E_{arrival} - E_1 \rvert$ such that $E_{arrival}$ = - 0.85 eV that is the energy of level 4. There is thus absorption from n = 1 to n = 4. This will lead to a total of 6 possible emission lines. However, among them, only two belong to the visible domain (1.55eV<Visible<3.1eV) that belong, for hydrogen, to the Balmer's series (E_4-E_2=2.55ev et E_3-E_2=1.89ev). The only spectrum with only 2 lines is spectrum C.	Many of you have realized that there was absorption in this situation, but has omitted the information that the detector recorded *only lines in the visible domain*. By the way, there was some confusion on the transition during absorption: when describing the transition, it involves the transition from n = 1 to n = 4 , and not from n = 4 to n = 1!!!
c)	<u>Situation 3 :</u> The range of energy associated to the range of frequency is 11.60 eV ≤ E_{ex} ≤ 13 eV, thus an interval for the arrival level that is -2.00eV ≤ $E_{arrival}$ ≤ - -0.60eV. Thus absorption occurs with two possible transitions: from n = 1 to n = 3 and from n = 1 to n = 4. This will lead to the same number of emitted lines as in situation 2, and thus the same 2 transitions than belong to the visible domain: from n = 4 to n = 2, and from n = 3 to n = 2. Thus same spectrum with only 2 lines : spectrum C.	Same comments as before
d)	E_4-E_2=2.55eV, thus using the provided equation, λ_{4to2}= 486.3nm E_3-E_2=1.89eV, thus using the provided equation, λ_{3to2}= 656.1 nm	