Lesson: POLYELECTRONIC ATOMS

PROBLEM SHEET: QUESTIONS

1. (♦◊◊) According to the results by Clementi and Raimondi the effective nuclear charges of the different orbitals for the ten first elements are

Átomo	$1s$	$2s$	$2p$
H	1		
He	1.6888		
Li	2.691	1.279	
Be	3.685	1.912	
B	4.680	2.576	2.421
C	5.673	3.217	3.136
N	6.665	3.847	3.834
O	7.658	4.492	4.453
F	8.650	5.128	5.1
Ne	9.642	5.758	5.758

Using these data,

a) Calculate the electronic energy of Lithium

b) Calculate $\langle r \rangle$ for the most external electron of the elements of the second period.

c) Calculate $\langle r \rangle$ for the $2s$ orbital of the elements of the second period.

2. (♦♦◊) Calculate using the data of the previous exercise the energies of the $1s$ and $2s$ electrons of the lithium atom. Let us consider that the Lithoium atom is described using the model of a particle in a one-dimensional box. Calculate the length of the box so that the energy difference obtained using that model is identical to the previous one. Compare the length obtained with the average values ($\langle r \rangle$) for the $1s$ and $2s$ electrons calculated using the effective nuclear charges.

3. (♦♦♦) The first ionization potential of the A element is the energy required to extract one electron from the atom A

$$A \rightarrow A^{+} + e^{-},$$

the second ionization potential corresponds to the loss of a second electron

$$A^{+} \rightarrow A^{2+} + e^{-},$$

and so on.

Search the experimental values of the 16 ionization potentials of sulfur and make a plot. Discuss the trends in terms of the electronic configurations of the successive ions.

(**Hint**: Calculate the differences beteween consecutive ionization potentals to detect the most stable configurations.)

Dificulty level: (♦◇◇) Easy, (♦♦◇) Normal, (♦♦♦) To think a bit.

PROBLEM SHEET: SOLUTIONS

Question 1 ⇒ (a) -202.5 eV.

(b) $\langle r \rangle$ = 2.48, 1.66, 1.09, 0.84, 0.69, 0.59, 0.52 y 0.46 Å.

(c) $\langle r \rangle$ = 2.48, 1.66, 1.23, 0.99, 0.83, 0.71, 0.62 y 0.55 Å.

Question 2 ⇒ $E_{1s} = -98.48$ eV, $E_{2s} = -5.56$ eV, $l = 1.101\text{Å}$, $\frac{1}{2}(\langle \hat{r} \rangle_{1s} + \langle \hat{r} \rangle_{2s}) = 1.39\text{Å}$