

Lesson: POLYELECTRONIC ATOMS

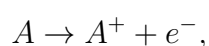
PROBLEM SHEET: QUESTIONS

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

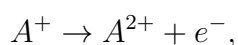
Átomo	1s	2s	2p
H	1		
He	1.6888		
Li	2.691	1.279	
Be	3.685	1.912	
B	4.680	2.576	2.421
C	5.673	3.217	3.136
N	6.665	3.847	3.834
O	7.658	4.492	4.453
F	8.650	5.128	5.1
Ne	9.642	5.758	5.758

Using these data,

- Calculate the electronic energy of Lithium
 - Calculate $\langle r \rangle$ for the most external electron of the elements of the second period.
 - 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 Lithium 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



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



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 between consecutive ionization potentials to detect the most stable configurations.)

Difficulty level: (◆◆◆) Easy, (◆◆◆) Normal, (◆◆◆) To think a bit.

PROBLEM SHEET: SOLUTIONS

Question 1 \Rightarrow (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 \AA .

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

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