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The Bohr atomic model, the first ionization energy and the effective nuclear charge to element 119: understanding the periodic trends along group 1

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Abstract. In the present work, by using and empirical equation involving the“last” ionization energy for group 1 elements, the first ionization energy to element 119 is calculate as 4.12 eV. Such value is in good agreement with previously calculated ones. Furthermore, it is shown that, for group 1 elements, the second IE/first IE ratio tends to remain constant as Z increases, even for Fr and element 119, for which the relativistic contributions are pronounced. The effective nuclear charge to element 119 was calculated as 4.40 and for francium, Z_{eff} = 3.83.

Keywords: Element 119; Ionization energy; Super-heavy elements; effective nuclear charge

INTRODUCTION

As is well known, in the Bohr atomic model, the electron energy (in eV units) in a given energy level is given by:

$$E = Z^2\ 13.6/n^2 \qquad (1)$$

where n is an integer number (the main quantum number, we say today).

Of course, it is also well known that the Bohr model don´t work well to atoms with higher atomic numbers. In fact, it works very well only to hydrogen (Z =1).

However, if we use Eq. (1) to calculate the third ionization energy to Li (Z=3) we obtain 122.40 eV as result, in very good agreement with the experimental value of 122.45 eV [1]. If we apply Eq.(1) to calculate the 7th ionization energy of nitrogen, we obtain 666.4 eV, once again in very god agreement with the experimental value: 667.05 eV [1].

Of course, such achievements are not a surprise, since if we remove "all but one" electrons from a given neutral atom, we will be left with a system composed of a nucleus and one electron, such as the hydrogen atom.

For such application, Eq. (1) works well even for higher Z values atoms, such as nickel (Z =28), for which Eq. (1) give as a 10,662.4 eV energy to remove the last electron, against a reference value of 10,775.48 eV [2].

There is, in principle, no reason to believe that Eq. (1) would not work equally well for heavy elements, and even for super-heavy ones. Therefore, we will use Eq.(1) as a starting point to calculate the first ionization energy of element 119, comparing the value calculated here with the values available in the literature.

METHODOLOGY

Reference values [1] for the first ionization energies for K, Rb and Cs were plotted as a function of the energy required to remove the "last electron" from the same elements (calculated using Eq. 1). The graph obtained was a straight line (r = 0.9999), thus obtaining an empirical equation:

$$IE = -1{,}226 \times 10^{-5} E + 4.403 \qquad (2)$$

were IE is the first ionization energy and E is the "last" ionization energy, such as calculated by using Eq. (1) .

To obtain Eq. (2), Li and Na were left out as they are the lightest elements in the group.

Perhaps for some people, such an approach may seem too "primitive", but it has been verified that, when it comes to super-heavy elements, a simple approach can lead to effectively excellent results [3,4].

By using Eq. (2), we calculate to element 119 an IE value of 2.04 eV. However, in the case of heavy elements and, even more so, for super-heavy ones, relativistic contributions must necessarily be taken into consideration [5].

RESULTS AND DISCUSSION

To Z = 119, a Lorentz factor of 2.02 can be calculated, since $\gamma = 1/\{1-[(Z/137)^2/c^2]\}^{1/2}$. Hence, a value of 2.04 x 2.02 = 4.12 eV can be calculate to the first ionization energy of element 119, in very good agreement with the 4.04 eV previously calculated value, based on absolute hardness [4]. Even if element 119 is treated as a calcium cluster [6], first IE values ranging from 3.76 to 5.68 eV are obtained.

The result obtained is in a logical order of periodic variations. Let's see: The first ionization energies (eV) to Li, Na, K, Rb and Cs are, respectively [1]: 5.59, 5.14, 4.34, 4.18 and 3.89, following the logic that ionization energy decreases as we "descend" along the group, just as we learned in high school.

However, the first ionization energy of francium increases (compared to cesium) to 4.07 eV, reflecting the observed relativistic contraction in its atomic radius. Thus, the calculated value of 4.12 eV for element 119 is following this increasing trend, as the relativistic contribution become even more pronounced, with increasing Z values.

Based on the calculated IE value, the effective nuclear charge to element 119 can be calculated as: 8 $(IE/13.6)^{1/2}$ = 4.40, and for francium, Z_{eff} = 3.83.

The curve shown in Figure 1 is a plot of the second IE/first IE ratios as a function of the atomic number (Z) from Na to element 119. From Na to Cs, the employed first and second ionization energies are reference values [1]. To francium, the first ionization energy employed was a reference value [1] and the second a previously calculated one [4]: Li = 75.64/5.59 = 14.03; Na = 47.29/5.14 = 9.2; K = 31.63/4.34 = 7.29; Rb = 27.29/4.18 = 6.53; Cs = 23.16/3.89 = 5.96; Fr = 23.80/4.97= 5.85; Element 119= 20.72/4.12 = 5.03.

As can be observed, the second IE/first IE ratio tends to remain constant as Z increases, even for Fr and element 119, for which the relativistic contributions are pronounced.

As previously verified to the period 7 elements [7], the IE values can exhibits "ups and downs" along the period (and, in the present study, along a group) taking into account that for some elements, the Z_{eff} contributions prevails whereas for another, the prevalence is of the relativistic factor, γ. As we can see by analyzing the curve in Figure 1, these factors tend to "equalize" as Z increases.

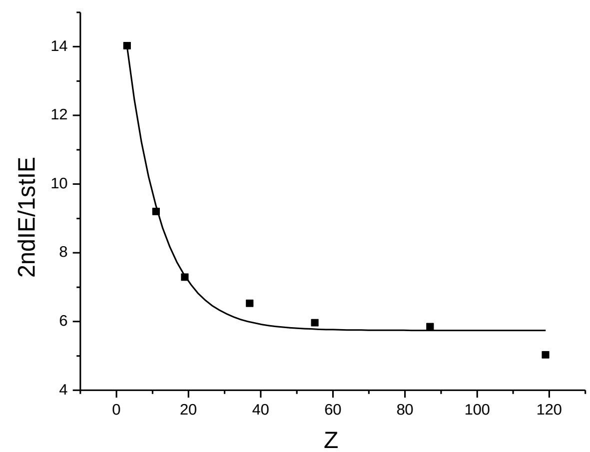

Figure 1. Second IE/first IE ratios as a function of the atomic number (Z) from Na to element 119.

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