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Research Article

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Estimating the Fermi Energies and Work Functions for the Super Heavy Elements 119 and 120 by using Cationic Absolute Hardness

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Abstract In the present work, is shown that here is a straightforward relationship between the absolute hardness for the mono or dication and the Fermi energy for group 1 and 2 elements. The absolute hardness (eV) for 119^+ and 120^{2+} are estimated as 8.34 and 17.14, respectively. By using such values and empirical equations, the Fermi energies (eV) to the elements 119 and 120 were calculated as 1.48 and 4.20, respectively. By using such E_F values and an equation derived by Halas [9], the work functions (eV) for the elements 119 and 120 were calculated, respectively, as 1.77 and 2.17.

Keywords Fermi energy, work function, superheavy elements, element 119, element 120, absolute hardness

Introduction

Taking into account that, for superheavy elements, direct measurements of their chemical and physical properties are difficult or even impossible tasks, a lot of efforts have been made in order to estimate/calculate the properties of such elements, such as their formation enthalpies [1].

The present work is inserted in this context and is dedicated to estimate the Fermi energies and work functions for the elements 119 and 120.

Methodology, Results and Discussion

Using the ionization energy values [2,3] absolute hardness values (eV) for Li^+ (35.12), Na^+ (21.08), K^+ (13.64), Rb^+ (11.56), Cs^+ (9.61); Be^{2+} (67.84), Mg^{2+} (32.56), Ca^{2+} (19.52), Sr^{2+} (15.93) and Ba^{2+} (13.66) were calculated. Such values, as well as the Fermi energies (eV) to groups 1 and 2 elements [4] are summarized in Table 1.

Table 1: Absolute hardness and Fermi energies for group 1 and 2 cations/elements

Specie/property	η^+ or η^{2+} /eV	ϵ_F/eV
Li		4.72
Li^+	35.12	
Na		3.23
Na^+	21.08	
K		2.12
K^+	13.64	
Rb		1.85
Rb^+	11.56	
Cs		1.58
Cs^+	9.61	
Be		14.3

Be^{2+}	67.84	
Mg		7.08
Mg^{2+}	32.56	
Ca		4.69
Ca^{2+}	19.52	
Sr		3.93
Sr^{2+}	15.93	
Ba		3.64
Ba^{2+}	13.66	

When the Fermi energy (eV) for the group 1 elements are plotted as function of the absolute hardness (eV) to the respective monocations, the curve shown in Figure 1 is obtained, from which Eq. (1) (r = 0.9971) was derived:

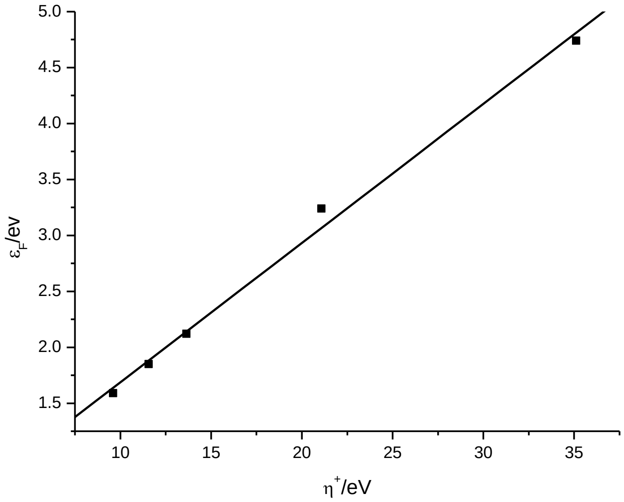

***Figure 1**: Fermi energies as a function of monocation absolute hardness for group 1 elements*

$$E_F = 0.124\ \eta^+ + 0.444 \quad (1)$$

When the Fermi energy (eV) for the group 2 elements are plotted as function of the absolute hardness (eV) to the respective dications, the curve shown in Figure 2 is obtained, from which Eq. (2) (r = 0.9997) was derived:

$$E_F = 0.198\ \eta^{2+} + 0.807 \quad (2)$$

The absolute hardness for 119^+ was previously estimated [5] as 8.34 eV.

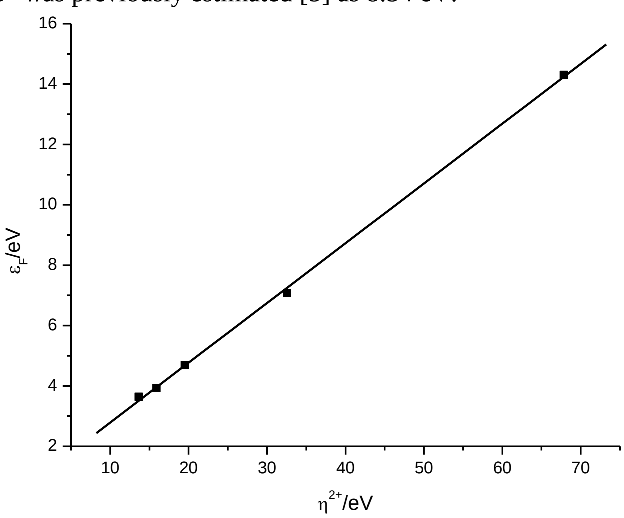

Figure 2: Fermi energies as a function of dication absolute hardness for group 2 elements

In order to know the absolute hardness for 120^{2+} we need to know the second and third ionization energies for element 120. The second IE have was calculated as 11.137 eV, by relativistic quantum chemical methods [6].

There are not, in the literature, a value for the third ionization energy of element 120. Hence, it was estimated as follows: the third ionization energies for Mg, Ca, Sr and Ba were plotted as a function of the second ionization energies, providing the curve shown in Figure 3 (r= 0.9967), from which Eq. (3) was derived:

$$IE_3 = 8.730\ IE_2 - 51.816 \quad (3)$$

Using Eq. (3) and the second IE for element 120 [6] its third ionization energy was calculated as 45.41 eV. Using the third and second IE values, the absolute hardness for 120^{2+} was calculated as 17.14 eV.

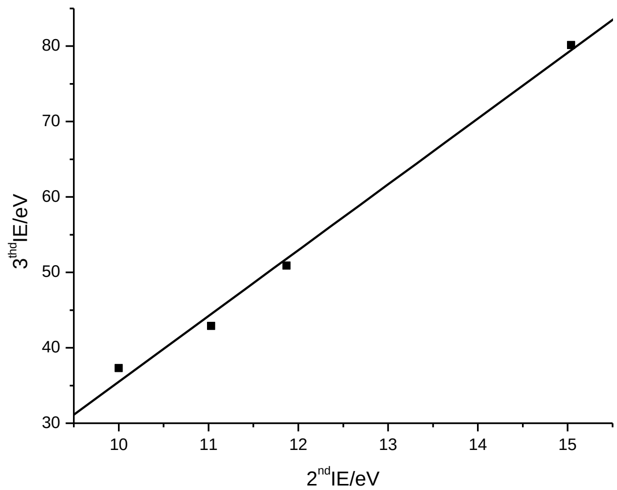

Figure 3: Third ionization energy as function of the second ionization energy for Mg, Ca, Sr and Ba

Applying the respective absolute hardness values in Eq. (1) and (2), the Fermi energies for elements 119 and 120 were calculated. The obtained results are summarized in Table 2.

Table 2: Absolute hardness to the cations and Fermi energies and work functions for elements 119 and 120

Specie/property	η^+ or η^{2+} /eV	ϵ_F/eV	φ/eV
119		1.48	1.77
119^+	8.34		
120		4.20	2.17
120^{2+}	17.14		

As can be verified, the Fermi energy for 119 is very close to the Fermi energy to Cs, and the E_F value to element 120 is higher than the value for barium. Both facts are in total agreement with a foreseeable relativistic contraction for superheavy elements [7,8].

The absolute hardness is defoned as: η = (IE-EA)/2 (IE= ionization energy; EA = electron affinity). Since, with very good approximation, E_{HOMO}= -IE and E_{LUMO}= -EA, then, η = (E_{LUMO} - E_{HOMO})/2.

Hence, Eq.(1) became:

$$E_F = 0.124\ [(E_{LUMO} - E_{HOMO})/2] + 0.444 \quad (4)$$

Is necessary to remember that we are talking here of the frontier orbitals for the cations, not simply the neutral atoms.

On the other hand,

$$E_F = \frac{\hbar^2}{2m}\left(\frac{3\pi^2 N}{V}\right)^{2/3} \quad (5)$$

Hence:

$$\frac{\hbar^2}{2m}\left(\frac{3\pi^2 N}{V}\right)^{2/3} = 0.124\ [(E_{LUMO} - E_{HOMO})/2] + 0.444 \quad (6)$$

Since, in such equation, only (N/V) and (E_{LUMO} - E_{HOMO}) are variables, we have, of course, a straightforward relation between the concentration (also called "density") of (free) electrons and the energy gap of the frontier orbitals, and they are directly proportional. Of course, an analogous equation can be derived for group 2 elements.

This conclusion is in agreement with the fact that E_F can be correlated with the respective work functions [9], and the work function is inversely proportional to E_F.

Halas [9] have shown that

$$\varphi = (43.46\ \alpha)/(r_S^{3/2} E_F^{1/2}) \quad (7)$$

were φ is the work function (eV), α is a parameter scaling factor (that was assumed to be equal to unity for all elements except the alkalimetals, Ca, Sr, Ba, Ra and Tl, for which it was assumed to be equal to 0.86) and $r_S$is the electron density parameter, expressed in the units of Bohr radius.

Using Eq. (7) and the previously calculated E_F values, the respective work functions, shown in Table 2, were calculated. For both elements, α = 0.86, and the respective r_s values were obtained, by extrapolation, as 6.70 and 4.14, for the elements 119 and 120, respectively.

Using the calculated Fermi energies for elements 119 and 120, another parameters of the Fermi gas (electrons concentration, Fermi velocity, etc.) can, of course, be calculated.

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