**Research article**

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# Estimation of Clementi effective nuclear charges and ionization energies for superheavy elements: explaining the variations for IE along period 7

**Robson Fernandes de Farias**

Universidade Federal do Rio Grande do Norte, Cx. Postal 1664, 59078-970 Natal-RN, Brazil

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**ABSTRACT:**

*In the present work, by using empirical equations, the Clementi effective nuclear charges ($Z_{eff}$) for superheavy elements are estimated as: Rf = 12.00, Cn = 14.47, Fl= 16.55, Mc= 17.72, Lv= 18.67, Ts= 19.73, Og= 20.81 and to the element 120= 12.64. It is verified that there are very close relationships between the estimated $Z_{eff}$ and the theoretical or experimental ionization energies for the considered elements: to Rf, Og, Ts and Lv, IE ≈ $Z_{eff}/2$. To Fl and the element 120, IE ≈ $Z_{eff}/3$. To Mc, IE ≈ $Z_{eff}/4$ and to Cn, IE ≈ $Z_{eff}$. The IE values were also calculated by using the empirical equation $E_n= -[(13.6\ eV)\ (Z_{eff}^2/n^2)]/\ 4\gamma$, where $\gamma = 1/[1-((Z/137)^2/c^2)]^{1/2}$. The obtained results are in good agreement with relativistic quantum chemical values from literature [4-7]. For period 7 elements, is shown that $IE_{(Rel\cdot)} = (6.626 \times 10^{-2}\ Z_{eff}^2/\gamma) - 4.434$, and so, that there are two competitive and opposite contributions as Z increases: to $Z_{eff}$ and γ. Such opposing contributions explain why the IE values exhibits "ups and downs" along the period. It is shown, from Fl to Og, that the IE values are related by the equation: IE = 1.118 p + 8.344, where p is the number of electrons in the 7p shell. Using such equation, the IE for the element 113 is calculated as 9.46 eV.*

**KEY WORDS:** Superheavy elements, ionization energy; Clementi effective nuclear charge; relativistic contraction; empirical equation.

## INTRODUCTION:

The search for new chemical elements have resulted in the discovery of the elements 111-118, with some works dedicated to investigate/estimate/predict the properties of such elements [1, 2]. Since their chemical and physical properties are difficult of even impossible to be accessed/measured directly, the so-called superheavy elements have been the subject of a lot of theoretical investigations.

*** Corresponding author**

Robson Fernandes de Farias
Email: robdefarias@yahoo.com.br

 

The present work is inserted in this context, and is dedicated to estimate the Clementi effective nuclear charges [3, 4] for some superheavy elements: Rutherfordium (Rf), Copernicium (Cn), Flerovium (Fl), Moscovium (Mc), Livermorium (Lv), Tennessine (Ts), Oganesson (Og) and the element 120. Such estimated $Z_{eff}$ are employed to estimate the first ionization energies for these elements, in order to obtain information/insights about the electronic properties of such elements. The obtained results are compared with relativistic quantum mechanical calculations and experimental values from literature [5-8].

**METHODOLOGY:**

The employed method was a very simple one: to obtain the best and simpler correlation between Clementi effective nuclear charged and atomic number, and, by extrapolation, to estimate the Zeff for superheavy elements. Then, by using such estimated Zeff values, correlate then with another empirical equations, relating Zeff and ionization energies.

**RESULTS AND DISCUSSION:**

Plotting the Clementi [3,4] nuclear effective charge ($Z_{eff}$) as function of Z, the following empirical equations are obtained, for groups 1,4, 12, 14, 15, 16, 17 and 18 of the periodic table:

$Z_{eff}$ = 0.094Z+1.364 (r= 0.9900; group 1) (1)

$Z_{eff}$ = 0.087Z+2.944 (r= 0.9949; group 4) (2)

$Z_{eff}$ = 0.102Z+3.048 (r= 0.9970; group 12) (3)

$Z_{eff}$ = 0.122Z+2.644 (r= 0.9972; group 14) (4)

$Z_{eff}$ = 0.127Z+3.114 (r= 0.9973; group 15) (5)

$Z_{eff}$ = 0.130Z+3.590 (r= 0.9965; group 16) (6)

$Z_{eff}$ = 0.134Z+4.054 (r= 0.9968; group 17) (7)

$Z_{eff}$ = 0.138Z+4.522 (r= 0.9970; group 18) (8)

By using therespective equations, the Clementi $Z_{eff}$ to Rf, Cn, Fl, Mc, Lv, Ts, Og and the element 120, shown in Table 1, were calculated. Also in Table 1 are shown the theoretical and, when available, experimental first ionization energies (eV) for these elements [5-8].

Table 1.Estimated Clementi $Z_{eff}$ and first ionization energies (eV) for some superheavy elements.

| Element | Z | $Z_{eff}$ | $Z_{eff}/2$ | IE/eV (Theor.) | IE/eV (Exp.) |
|---|---|---|---|---|---|
| Rf | 104 | 12.00 | 6.00 | _ | 6.00[a] |
| Cn | 112 | 14.47 | 7.24 | 11.48[b] | _ |
| Fl | 114 | 16.55 | 8.28 | 5.59[b] | _ |
| Mc | 115 | 17.72 | 8.86 | 4.80[c] | 5.2[c] |
| Lv | 116 | 18.67 | 9.34 | 7.88[e] | _ |
| Ts | 117 | 19.73 | 9.87 | 8.63[e] | _ |
| Og | 118 | 20.81 | 10.41 | 10.08[b] | 9.81[d] |
| 120 | 120 | 12.64 | 6.32 | 4.90[b] | _ |

[a]Experimental value, available at the Royal Society of Chemistry website: http://www.rsc.org/periodic-table;[b]ByHartree-Fock, scalar relativistic spin free method (Ref. 5); [c](Ref.6); [d]Experimental value (Ref. 7,8);[e]Values calculated by using the data from Ref. 7,8.

As can be verified, for Rf, Og, Ts and Lv, IE $\approx Z_{eff}/2$. To Fl and the element 120, IE $\approx Z_{eff}/3$. To Mc, IE $\approx Z_{eff}/4$ and to Cn, IE $\approx Z_{eff}$. Taking into account the uncertainty involved in the calculation of the ionization energy for superheavy elements, the found relationships can be considered quite good. Anyway, it is clear that there is a very close relationship between the ionization energies and the estimated Clementi effective nuclear charge values.

Since from Rf to Og, the Z, and, of course, $Z_{eff}$ values increases, seems natural to suppose that the IE values must also progressively increases. Hence, the "ups and downs" in the IE theoretical values [5-8] seems, in a first moment, unnatural, requiring an explanation.

Plotting the IE for groups 1,4, 12, 14, 15, 16, 17 and 18 of the periodic table [9] as function of the Clementi [3,4] effective charge ($Z_{eff}$), the following empirical equations are obtained:

$$IE = 0.029Z_{eff} + 3.708 \text{ (r = 1.000; group 1)} \quad (9)$$

$$IE = 0.070Z_{eff} + 6.178 \text{ (r = 1.000; group 4)} \quad (10)$$

$$IE = 0.486Z_{eff} + 5.016 \text{ (r = 1.000; group 12)} \quad (11)$$

$$IE = -0.092Z_{eff} + 8.536 \text{ (r = 0.9996; group 14)} \quad (12)$$

$$IE = -0.425Z_{eff} + 12.917 \text{ (r=0.9999; group 15)} \quad (13)$$

$$IE = -0.228Z_{eff} + 11.594 \text{ (r = 0.9948; group 16)} \quad (14)$$

$$IE = -0.458Z_{eff} + 15.826 \text{ (r = 0.9967; group 17)} \quad (15)$$

$$IE = -0.548\,Z_{eff} + 19.324 \text{ (r = 0.9920; group 18)} \quad (16)$$

By using the respective equations, IE to Rf, Cn, Fl, Mc, Lv, Ts, Og and the element 120, shown in Table 2, were calculated. The calculated values are compared with theoretical relativistic values from literature [5-8].

Table 2.First ionization energies (eV) for some superheavy elements.

| Element | Z | $Z_{eff}$ | γ | IE/eV (Eq.9-16) | IE/eV (Eq. 17) | IE/eV (Theor.)[a] |
|---|---|---|---|---|---|---|
| Rf | 104 | 12.00 | 1.536 | 7.02 | 6.50 | 6.00[b] |
| Cn | 112 | 14.47 | 1.736 | 12.05 | 8.37 | 11.48 |
| Fl | 114 | 16.55 | 1.803 | 7.01 | 10.54 | 5.59 |
| Mc | 115 | 17.72 | 1.840 | 5.39 | 11.84 | 4.80 |
| Lv | 116 | 18.67 | 1.879 | 7.34 | 12.87 | 7.88 |
| Ts | 117 | 19.73 | 1.922 | 6.79 | 13.56 | 8.63 |
| Og | 118 | 20.81 | 1.968 | 12.40 | 15.27 | 10.08 |
| 120 | 120 | 12.64 | 2.073 | 4.07 | 4.09 | 4.90 |

[a]Relativistic quantum chemical calculations (Ref. 5-8); [b]Experimental value, available at the Royal Society of Chemistry website: http://www.rsc.org/periodic-table.

The IE were also calculated by using the empirical equation:

$$E_n = -[(13.6\text{ eV})(Z_{eff}^2/n^2)]/4\gamma \quad (17)$$

Where n is the main quantum number for the considered electron and $\gamma = 1/[1-((Z/137)^2/c^2)]^{1/2}$, a correction factor introduced to take into account the relativistic effects/contributions for superheavy elements [10]. As can be verified from Table 2 data, the results obtained by extrapolation (Eq. 9-16), provide results in very good agreement with relativistic quantum chemical calculations [5-8]. Furthermore, to Rf and the element 120, Eq. (17) provides results in very good agreement with relativistic quantum chemical data.

Must be pointed out that, in deriving Eq. (9), (10) and (11), only the two heavier elements of each group was considered (this is the reason why r = 1.000). Such choice was made in order to make sure that the obtained equations were suitable for the heaviest element of the group (the superheavy element), that is, the derived equations includes the relativistic contraction observed for such elements [10]. When plotted as function of the ionization energies calculated by using Eq. (17), the relativistic quantum chemical ionization energies [5-8], for Fl, Lv, Ts and Og produces the curve shown in Figure 1 (r = 0.9991), and the equation:

$$IE_{(Rel.)} = 0.955\, IE_{(Eq.17)} - 4.434 \quad (18)$$

Making equals Eq. (17) and (18), and with n =7, we have:

$$IE_{(Rel.)} = (6.626 \times 10^{-2} Z_{eff}^2/\gamma) - 4.434 \quad (19)$$

Eq. (19) shows that higher $Z_{eff}$ elements have higher IE, and that, in the same period of the periodic table (elements with the same n), higher $\gamma$ values are related with lower IE. Since $\gamma$ increases with the increase of Z, and $Z_{eff}$ also increases as Z increases, there are two competitive and opposite contributions as Z increases: to $Z_{eff}$ and $\gamma$.

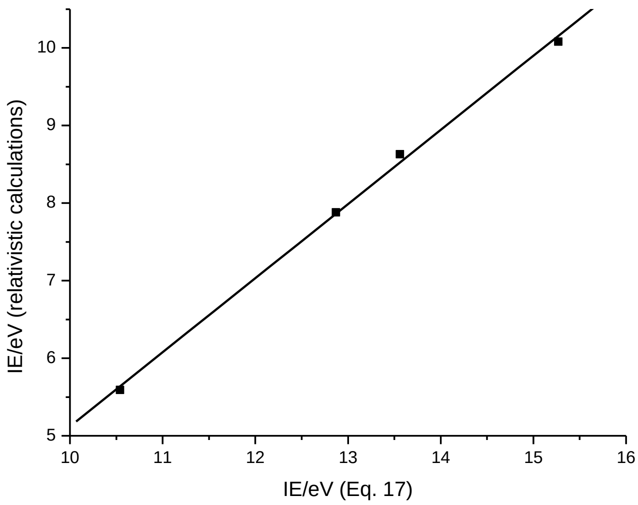


Figure 1.Relativistic ionization energies as function of the ionization energies calculated by using Eq. (17).

Such opposing contributions explain why the IE values exhibits such "ups and downs" along the period. For Cn and Og, the $Z_{eff}$ contributions prevails (higher IE values) whereas for Fl and Mc, the relativistic factor $\gamma$ prevails (lower IE values).

A most profound explanation for such facts comes from the electronic configurations: Cn and Og are closed shell elements: [Rn] $5f^{14}6d^{10}7s^2$ and [Rn] $5f^{14}6d^{10}7s^27p^6$, respectively. On the other hand, Fl and Mc exhibits incomplete p shells: [Rn] $5f^{14}6d^{10}7s^27p^2$ and [Rn] $5f^{14}6d^{10}7s^27p^3$, respectively. From Mc to Ts, the 7p level is been progressively completed and, consequently, the $\gamma$ contribution increases in a minor extent than the $Z_{eff}$ contribution, and such fact is related with the progressive increase in the IE values from Mc to Ts.

In figure 2 is shown the IE as function of the number of electrons in the 7p shell, from Fl to Og. The obtained curve (r = 0.9916), provides the equation:

 

IE = 1.118 p + 8.344 (20)

Where p is the number of electrons in the 7p shell. Using Eq. (20), an ionization energy of 9.46 eV can be calculated to element 113. Such value is, I believe, more reliable than the 7.31 eV previously estimated [11].

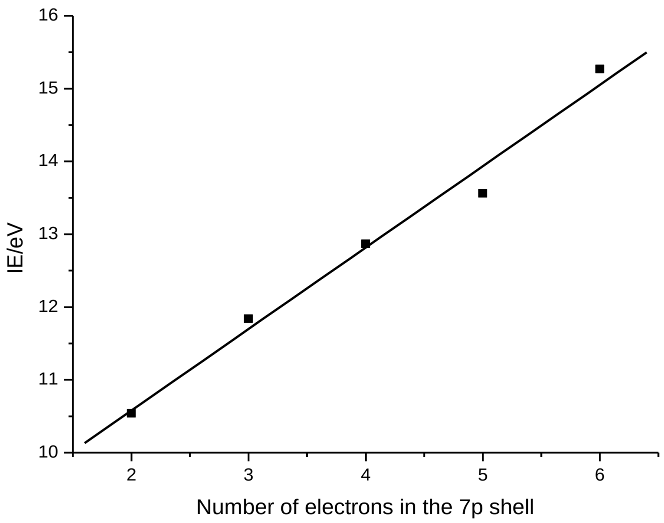


Figure 2. Ionization energies as function of the number os electrons in the 7s shell, from Fl to Og.

**CONCLUSION:**

The obtained results show that, by using very simple empirical equations, it is really possible to estimate the ionization energies for superheavy elements. Such obtained values are in very good agreement with reported values from literature, obtained by very sophisticated relativistic quantum chemical calculations.

**REFERENCES:**

1) R.F. de Farias, Chem. Phys. Lett., 667 (2017) 1.
2) R.F. de Farias, Chem. Res. J., 2(3) (2017) 108.
3) E. Clementi, D. L., J. Chem. Phys., 38 (1963) 2686.
4) E. Clementi, D. L. Raimondi, W. P. Reinhardt, J. Chem. Phys., 47 (1967) 1300.
5) C. Thierfelder, T. Schwerdtfeger, A. Koers, A. Borchevsky, B. Fricke, Phys. Rev. A 80 (2009) 022501.
6) O.L. Keller Jr., C.W. Nestor Jr., J. Phys. Chem., 78 (19) (1974) 1945.
7) J. Emsle,Elements, Mir, Moscow, 1993.
8) L.D. Landau, E.M. Lifshitz, Quantum mechanics. Non-relativistic theory. Butterworth-Heinemann, Burlington, 2003.
9) http://www.rsc.org/periodic-table.
10) J. Leszczynski, *Relativistic methods for chemists*, Springer, New York, 2010.
11) D.C. Hoffman, D.M. Lee, V.Pershina, Valeria, Transactinides and the future elements". In Morss; Edelstein, Norman M.; Fuger, Jean. *The Chemistry of the Actinide and Transactinide Elements* (3rd ed.), Springer, Dordrecht, 2006.

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