ARTICLE 09 ELECTRON PROBABILITY WITH NIN COUPLING IN n>2 AND NECESSARY NIN RELATIONSHIPS **Javier Silvestre** (eeatom.blogspot com)

ABSTRACT

This is 9th article of 24 dedicated to atomic model based on Victoria equation (Articles index is at end). First part continues electron density study [6,8] with atoms in Groups I, II and from XIII to XVIII (s and p blocks) whose n principal quantum number is higher than 2. Fundamental difference lies in Origin Electronic System MON (OES MON), which decreases as n increases (P37 [6]). Another factor that affects to lesser extent is Ionization Energy (IE) decrease when n increases. As in articles past, IE is given by [9] as Initial Energy (E_0) [1] and Maximum Probability radius to compare with contributed by NIN coupling is given by [10] and [11].

In the second part C_{POTI-AL} division and value are indicated and P44 Necessary NIN Relationships is introduced as one line to be deepened and implies that Electronic Systems values [6-8] follows trends along nuclear charge.

KEYWORDS

NIN coupling in n>2, Electron Probability, Maximum Probability, OES, BES, Necessary NIN relationships, Victoria Equation.

INTRODUCTION

A extern electronic extreme (EE_A) is indicated with a suffix $(r_A, H_A \text{ or } c_A)$, B intern with b suffix $(r_B, H_B \text{ or } c_B)$ and i suffix is used to both electronic extremes (EE_i). Suffixes B (Born) and O (Origin) appear from BES and OES concepts [6]. All abbreviations are compiled, in conjunction with those included in [6,8], at article end.

Based on [8] where $n=2$ Probability (P_i) curves coupling is studied by NIN coupling (P34 [6]), n>2 is going to be developed. To reach this NIN coupling, energy radial distribution must be known by Victoria Equation [1], right-angled triangle relation must be conformed by two sides (orbital circumference (c_i) and circular orbital height (H_i)) and hypotenuse or radial distance (r_i) [2] and P_i meaning as rotation time conditioned by Compaction Factor (CF) must be defined [3,6]. NIN coupling factors (Effective nuclear charge (z), C_{PEP} , C_{POTI} and MON) and Maximum P_i calculations seen in [6-8] for n=2 are applied for n>2.

Pⁱ curves for n=3

For n=3 and according to P37 [6], 3s OES MON is 20 for Group I of Alkali Metals (Na), half of that value, i.e. 10, for Group II of Alkaline earth metals (Mg) and Groups XIII to XVIII of p-block are all MON=4. MON reminder for all n according to P37 is in **Table 1**.

Figure 1 is P_i vs. r_i for A and B electronic extremes (EE_A and EE_B) of electrons with $3s²3p^y$ electronic configuration in outermost shell. Atoms in Figure 1 are Si, P, S and Cl. Pⁱ curves and Maximum Pⁱ radius (**Table 2**) are in agreement with [10] and [11] and are displaced to greater radial distance (ri) values. 3 methods employed for Maximum Probability calculation in Table 2 are the same as those used in [8]. Method that only considers outermost electron $(3p^y)$ is considered as first approximation whose deviation increases with n since maximum between extern (in this case, $3p^y$) and intern (now is $3s²$) is increasingly separated. Unless otherwise indicated, geometry and probability treated is that of the outermost lobes of electrons in extern shell (in this case are $3s²$ and $3p^y$ in n=3).

In Figure 1 and Table 2 is maintained what is seen in [8]:

- 1) NIN coupling for all atoms.
- 2) Pⁱ curve and Maximum Pⁱ become closer as z OES increases.

3) If all OES have $C_{PEP}=1$, P_i decreases as z OES increases:

 \uparrow Z OES $\rightarrow \downarrow$ P_i and P_i and Maximum P_i closer to nucleus

4) Maximum P_i is in agreement with [10] and [11].

Pⁱ curves for n=4

In p-block, MON variation from $n=3$ to $n=4$ is less than in step from $n=2$ to $n=3$ and greater in s-block (Table 1). This fact related to MON and similar IE [9] causes that Pⁱ curves and maximum of n=3 and n=4 are similar in p-block, and are displaced to greater r_i in s-block (**Table 3**). As in P_i vs. r_i representation for $n=3$ (Figure 1), outermost lobes are represented in **Figure 2**.

Table 3 data are compared according to method used in **Figure 3**. The only method that is slightly deviated is "P_i Maximum by extern electronic system (extern lobe)".

Pⁱ curves for n=5

Methods and trends follow same guidelines as in Pⁱ curves in the previous case as verified in **Table 4**.

CPOTI-AL for OES

CPOTI angular limit or CPOTI-AL (P32 [5]) is indicated for ns OES in **Table 5**. CPOTI-AL for Born Electronic System (BES in P36 [6]) can be approximated by (1) (P43 [6])

$$
(1) C_{POTI - B} = C_{POTI - O} \sqrt{\frac{(E_o)_B}{(E_o)_O}}
$$

C_{POTI-AL} continuous increase when OES z grows is broken in $n > 3$ by $(n-1)d$ intercalation and subsequent interspersed f-block. CPOTI-AL shows this increase with a nondiscontinuous curve for every n in p-block (**Figure 4**). C_{POTI-AL} for $n=2$ is also included with data from [7]. Continuity in the increase is broken when passing from s-block to pblock by interspersed blocks as has been commented and also for the same reason, within the same p-block Groups.

P44 Necessary NIN relationships

Probability factors included in lobe or Electronic System [6] have tendencies that are fulfilled through EE z.

P34 main consequence is that two different energies meet in $d \rightarrow \infty$ (EE birth point [1]) and geometric and probabilistic NIN couplings (GNC or PNC) are achieved on both d→∞ sides. This accomplishment simultaneously opens possibility and dilemma that any energy can comply GNC and PNC. "P44 Necessary NIN relationships" emerges as research branch to avoid dilemma and to select energy possible.

P44 variation of CPOTI-AL value and division is studied as introduction although are not the most sensible elements to energy variations. P44 variation is the studied element variation throughout Electronic System z.

CPOTI-AL P44: behaviour and sensibility

C_{POTI-AL} P44 behaviour has been seen in Table 5. Sensibility to OES Ionization Energy (OES IE) variation is now checked in **Figure 5**.

Figure 5 has two C_{POTI-AL} curves for 2s OES from Group XIII to XVIII. On the one hand, curve made with experimental IE and on the other, curve called " $N(+1\%$ IE)" which is experimental IE, but in the case of 2s Nitrogen IE has been increased by 1%. $R²$ of potential trend line falls with modified 2s Nitrogen IE and Nitrogen point is misaligned with trend line. For example, R^2 of three degree polynomial regression falls from 0.9999 to 0.9939.

CPOTI-AL division P44: behaviour and sensibility

ns OES C_{POTI-AL} divisions with $n=[2-5]$ are in **Tables 6 to 9**. As for $n=2$ [7], C_{POTI-AL} division undergoes sudden changes when MON is modified and is practically constant when MON does not vary (for example, p-block in a given n). "Practically constant" is actually a slight increase in accordance with OES z. This outstanding relationship between C_{POTI-AL} divisions and MON has not been seen in C_{POTI-AL} value (Table 5).

ns OES C_{POTI-AL} division with $z=1$ (i.e., and according to P14 [1], OES $z=1$ is Group I: Alkaline) has linear trends with R^2 =0.9997 for n=[2,5] (**Figure 6**) although is expected a curvature of said linearity towards point $(0,0)$ (MON=0 and C_{POTI-AL} division=0 when

n→∞). In fact, R^2 =1.000 for n=[2-4] and curvature is increased when n=6 is included in regression.

 $C_{POTI-AL}$ division sensitivity to IE variations is reduced due to this outstanding relationship with MON. **Figure 7** is Figure 6, but includes $\pm 10\%$ modification for 3s OES IE. This IE modification is very high and, although with a minor modification also there is trend alteration, there are elements that show a remarkable sensitivity to low IE variations (less than 0.1%). This high energy sensitivity is seen in third part (See Articles index at end)

All C_{POTI-AL} division vs. MON for OES from $z=1$ (Group I) to $z=8$ (Group XVIII) are in Figure 8. Tendencies for these new OES considered have greater curvature than if OES is from Group I (Figure 6) since their MON are inferior and are in the curvature expected zone towards point (0,0) previously commented. Block-p curves run approximately parallel and $\frac{\text{Division of C}_{\text{POTI-AL}}}{\text{ACOM}}$ ratio increases with OES z (**Figure 9**). MON -10% OES IE modification effect is easy to appreciate when being parallel curves. Said modification has been included in As (z=5 for its OES) in **Figures 10** and curve showing -10% OES IE alteration effect is "z=5 $(*)$ ".

BIBLIOGRAPHY

[1] Javier Silvestre. Victoria Equation - The dark side of the electron. (Document sent to vixra.org)

[2] Javier Silvestre. Electronic extremes: orbital and spin (introduction). (Document sent to vixra.org)

[3] Javier Silvestre. Relations between electronic extremes: Rotation time as probability and First Feliz Solution. (Document sent to vixra.org)

[4] Javier Silvestre. Feliz II the prudent: Probability radial closure with high order variable C_F . (Document sent to vixra.org)

[5] Javier Silvestre. Feliz III The King Major: Orbital filled keeping Probability electronic distribution. (Document sent to vixra.org)

[6] Javier Silvestre. Feliz IV Planet Coupling: Probability curves NIN coupling from origin electron. (Document sent to vixra.org)

[7] Javier Silvestre. NIN Coupling values in n=2 and Oxygen electronic density. Silvestre Valor 07. (Document sent to vixra.org)

[8] Javier Silvestre. Electron Probability with NIN coupling in n=2. (Document sent to vixra.org)

[9] Kramida, A., Ralchenko, Yu., Reader, J., and NIST ASD Team (2014). NIST Atomic Spectra Database (ver. 5.2), [Online]. Available:<http://physics.nist.gov/asd>

[10] S. Fraga, J. Karwowski, K. M. S. Saxena, Handbook of Atomic Data, Elsevier, Amsterdam, 1979.

[11] Desclaux JP. Relativistic Dirac-Fock expectation values for atoms with $Z = 1$ to Z $= 120$. Atom Data Nucl Data Tables 1973;12: 311-406.

Abbreviations List

Suffix indicates electronic extreme considered and i suffix is used to both electronic extremes (EE_i). Following Table indicates abbreviations used in this theory and its use in article in question is marked with X. 9 is present article. Jump from "Article 09" to "Article 20" is consequence of second part inclusion.

12

 $\overline{\mathbf{1}}$