ARTICLE 10 EXCITED ELECTRONS BY TORREBOTANA CENTRAL LINE TETE-VIC EQUATION Javier Silvestre <u>www.eeatom.blogspot.com</u>

ABSTRACT

This is 10th article of 24 dedicated to atomic model based on Victoria equation (Articles index is at end). Electron excited states are born referenced to central line denominated Torrebotana with origin always in the first Origin Electronic System (OES) of all atom: 1s [6,9]. This central line that defines energies and charges (z) for central excited states is given by Tete-Vic equation. Excited states are directed towards Torrebotana Central Line approaching when n and l of destination excited state increase.

Fist, Torrebotana Central Line application is centred in Beryllium case for which excited state energy is approaching Torrebotana as indicated above. Subsequently, other atoms are studied to corroborate what is seen in Be case and to discover trends in terms of Atomic Number (Z) that serve to open new research lines.

KEYWORDS

Tete-Vic equation. Torrebotana Central Line, z_{CT} (Zon Equation), excited state, Jump Energy (Ej).

INTRODUCTION

Theory introduction for electron excited states deals only sporadically with seen in electron of two electronic extremes [1,9], although ultimate goal is complete union of both theories. If initially Electronic Extreme Theory is opened with Victoria Equation to obtain radial distribution of energy, now Tete-Vic Equation creates distribution of energy and charge in base to the destiny.

Geometry and Probability of electronic extremes [2,9] are not yet employed, although some conclusions of such references are included as: P41 Electron charge (z) coupling and its relation between energy and charge belonging to NIN couplings [6], new vision of P14 dedicated to effective nuclear charge (z) [1] or the conceiving of 1s as origin of all other electronic extremes (Born Electronic System or BES) [6,9]. Abbreviations Table is at end article.

Torrebotana Central Line theory, from which excited states are explained, requires following postulates:

P45 Excited state charge (zct) in Torrebotana Central Line

Excited state charge (z_{CT}) in Torrebotana Central Line is ideal charge to which excited state are attracted to greater or lesser extent depending on destiny quantum numbers and is given by "Zon Equation"(1):

- $(1)z_{\rm ct} = \frac{z_{\rm s}^2}{n^2 z_{\rm o}}$
- z_s Start charge according to P46
- z_o 1s Origin charge according to P46
- n Principal quantum number of excited state

Formula implies that when $n \rightarrow \infty$, excited state charge (z_{CT}) tends to 0 and therefore is nucleus independent.

P46 non-excited electronic extreme charge

P46 is closely related to P14 titled: Effective nuclear charge in ns electron external lobe [1] postulating:

"In the simplest model, first electron (1s) interacts with all protons and z is equal to Atomic Number (Z). Nucleus loses one charge with this first electron. Therefore, second electron interacts with Z-1 nuclear charge and so on, third electron with Z-2, fourth electron with Z-3... Until the outermost electron interacts with only Z=1. However, the simplest model only occurs with external lobe of ns electron. Consequently, 2s electron in is outermost lobe has $z_{2s} = Z-2$ and, for example, z_{2s} for Li(I) and B(III) is 1 and 3 respectively. 3s electron Argon has z_{3s} (Ar) = Z-10=18-10=8. Subsequently, z is formulated for other electrons and internal lobe of ns electron as z coupling between them. This idea is part of NIN continuation introduced in P04." [1]

P14 application only for external lobe of ns electron is valid for NIN relations, Negative in Negative [6,9], but charge electrons have and that excited states feel is equal to that indicated in P14 and is the one used in Zon Equation (1). Consequently and for z_{CT} , effective nuclear charge is very simple to calculate since only whole units must be subtracted from initial charge. **Table 1** indicates P46 non-excited electronic extreme charge for Zon Equation in Boron example:

Table 1 - P46 non-excited electronic extreme charge for Zon (1) in Boro (Z=5)							
Electron1s $1s^2$ 2s $2s^2$ 2p							
Charge 5 4 3 2 1							

P47 Torrebotana Central Line: Tete-Vic Energy Equation

Tete-Vic Energy Equation (2) creates Torrebotana energetic central line, excited state centre and is the version of P41 Electron charge (z) coupling and its relation between energy and charge belonging to NIN couplings [6]. Now, excited state destiny energy (E_d) is used instead of E_B (Born Electronic System Energy).

E_d Excited state destiny energy

E_o OES Energy

$$(2)E_{d} = \frac{z_{ct}E_{o}}{z_{o}}$$

(2) is transformed into (3) by (1) and E_d is function of charge quotient with exponent equals to 2 (z_s (Start charge) and z_o (OES charge)) E_o (OES Energy) and n principal quantum number which also has exponent of 2. (3) is Tete-Vic Energy Equation based on E_d :

$$(3)E_{\rm d} = \frac{z_{\rm s}^2 E_{\rm o}}{z_{\rm o}^2 n^2}$$

Jump Energy (E_J) (4) is defined as energy that must be contributed to reach from state with lower energy or non-excited to excited state (E_d) . Non-excited energy is Ionization Energy (IE) if not indicated otherwise [1] and its value is contributed by [10]. Excited states energies are also taken from NIST Atomic Spectra Database Lines Data [11]. Where E_J is always positive because IE and E_d are negative and IE is always higher (in absolute value) than E_d .

(4)
$$E_j = E_d - IE = \frac{z_s^2 E_o}{z_o^2 n^2} - IE$$

From 1s² (Term ¹S; J=0) to 1snx

Torrebotana Central Theory goodness is checked in following figures and tables. For this, first any atom or ion is chosen (Beryllium), initial state or non-excited state $(1s^2 \text{ electron} \text{ in Be III: Term } ^1\text{S}; J=0)$ and final state or excited state that depending on quantum numbers of excited state can be many and have been selected one from each orbital quantum number (s, p, d and f) and indicated in **Table 2**.

Table 2 - Destiny or final states selected for jump in Be III (1s ² Term= ¹ S and J=0)						
Excited State	1sns	1snp	1snd	1snf		
Term J ${}^{1}S 0$ ${}^{1}P^{0} 1$ ${}^{1}D 2$ ${}^{1}F^{0} 3$						

Excited state charge (z_{CT}) in Torrebotana Central Line (1) is summarized in **Table 3** from Start charge ($z_s(1s^2 Be)=3$), 1s Origin charge ($z_o(OEs Be)=4$) and in function of destiny n.

Table 3 - I	Table 3 - Be Torrebotana Central Line Charge with start in $1s^2$ (z_{CT} ($1s^2$ Be)) (Till n=10)				
n	ZCT				
2	0,5625				
3	0,25				

4	0,140625
5	0,09
6	0,0625
7	0,04591837
8	0,03515625
9	0,02777778
10	0,0225

Reference energies [11] (E_k) are energy needed to reach excited states and are compared with Jump Energy (E_J) (4) (**Table 4**). Es, Ep, Ed and Ef are necessary energies to reach ns, np, nd and nf respectively (with Term and J indicated in Table 2 and 4).

Table 4 - E_k , E_j and z_{CT} for $1s^2$ Be till n=10						
			R	eference ene	rgies [11] (E	k)
n	ZCT	Ej	Es	Ep	Ed	Ef
			${}^{1}S 0$	${}^{1}P^{0} 1$	¹ D 2	${}^{1}F^{0}$ 3
2	0,5625	123,279523	121,6506	123,6685		
3	0,25	140,288787	139,8176	140,3985	140,2834	
4	0,140625	146,242029	146,054	146,2803	146,2387	146,2411
5	0,09	148,997530		149,0159	149,0042	148,997
6	0,0625	150,494345		150,5083		150,4939
7	0,04591837	151,396878		151,4014		
8	0,03515625	151,982656				
9	0,02777778	152,384263				
10	0,0225	152,671531				

Figure 1 shows energetic jumps from initial configuration of $1s^2$ Be (Term 1S; J=0). From Table 4 and considering that scale includes energetic interval [0,160] eV is possible to presage apparent overlap between Torrebotana Central Energetic Line (indicated by E_J) and reference energies (defined by four E_k curves). **Figure 2** reduces interval to [120,160] eV and is already possible to observe slight separation between Torrebotana Central Energetic Line and jump to 1s2s and to lesser extent with 1s2p.



Actual change (5) is a better way to verify differences between energetic curves (**Figure 3**):

(5) Actual Change = $AC = \Delta = E_J - E_k$

In this $1s^2$ Be case, four curves are referenced with the same Torrebotana Central Energetic Line, but in other occasions this fact does not occur (for example when different atoms are compared). In such cases may be useful to take into account the size of Torrebotana Central Energetic Line and use Relative Change (RC) whose formula including percentage (%RC) comes with (6):

(6)%RC =
$$\frac{(E_j - E_k)}{/IE/} * 100 = \frac{(E_j - E_k)}{-IE} * 100$$



Figure 4 is made from (6) % Relative Change. Both Figure 3 and 4, whose data are in **Table 5** and **Table 6** respectively (**Annex**), present clear trends:

a) Differences between E_J and E_k are small. $1s^2$ to 1s2s (¹S 0) has the biggest difference and is about $\approx 1\%$. Relative Change or Actual Change is not indicated as an error because it not really an error because Torrebotana Central is the Energetic Line at which energetic curves of excited states are attracted, but Torrebotana Central Energetic Line is not exact value of any E_k curve.

b) Differences, both relatives (6) and not (5), decrease as n increases.

c) Difference vs. n draw curves without discontinuities. This continuity is appreciated for 1sns and 1snp. For jumps to 1 higher (d and f orbital) is better to wait for higher % RC because now gives $RC \rightarrow 0$ and analysis is very conditioned to data or mechanisms not explained in this introduction.



d) Absolute value of Actual Change and % Relative Change decrease as orbital quantum number increase. This fact is especially clear with sequence: s > p > d. That is, as orbital quantum number increases, E_k curve is more attracted by E_J curve. For that reason, Ed or Ef curve should be chosen to have better idea of Torrebotana Central Energetic Line and not to make Es curve selection.

The same procedure followed with $1s^2$ Be is performed with $1s^2$ O (Term ¹S; J=0) to check for repeatability. Increase in z_0 and E_0 and generally decrease in number of data [11] is produced when z_s of electronic system is increased. All Ek>500 eV for $1s^2$ O (**Table 7**) and, although Actual Change (5) are somewhat superior (Table 5 and Figure 3 vs. **Table 8** and **Figure 5**), Percentage Relative Change (% RC) is lower at least in E_k with lighter behaviour: Es and Ep (Table 6 and Figure 4 vs. **Table 9** and **Figure 6**). Tables 7, 8 and 9 are in **Annex**.

The main lines complied by Be are continued with O:

a) Reference data curve are attracted to Torrebotana Central Energetic Line.

b) Attraction is accentuated when n and l increase.

c) Declines of energetic differentials in n function present morphology curve without discontinuities.



From 2s (Term ²S; J=1/2) to 1s²nd (Term ²D; J=5/2)

Once correct operation of Torrebotana Central Energetic Line has been seen for specific case of Be and O from start configuration $(1s^2 \text{ (Term }^1\text{S}; J=0))$ to excited states 1snx (x = s, p, d and f), other initial configuration must be studied to corroborate what has been

developed in previous point and possibility of a tendency as Atomic Number increases, and consequently z_s and z_o that conform z_{CT} according Zon equation (1), must be analyzed.

On the one hand, initial configuration is changed from $1s^2$ to 2s. On the other hand, atoms of second period are calculated and, in addition, distant atom such as Fe Z=26 is included in comparative.

Initial state is the one corresponding to $1s^22s$ configuration whose Term=²S and J=1/2, while final state is excited type state: $1s^2nd$ with Term=²D and J=5/2. Initial and Final states do not imply that is a direct step since interesting objective in this introductory article is to corroborate goodness of Torrebotana Central Energetic Line (E_J) with respect to curves created with reference data (E_k).

Figure 7 shows reference energy data [11] as Ed and Torrebotana Central Energetic Line (E_J) as Ej Li, Ej Be and Ej B for Lithium, Beryllium and Boron respectively. Positive conclusion is that both, Reference and Torrebotana curves, are superimposed.



Energetic curves comparison with disparate energetic jumps is improved if E_j or E_k (in this case, Ed) are divided by absolute IE value. Result is called referenced energy to IE and is indicated with suffix R (7) and (8):

(7)Referenced Jump Energy =
$$E_{j,R} = \frac{E_j}{-IE}$$

(8)Referenced Reference Energy =
$$E_{k,R} = \frac{E_k}{-IE}$$

If E_J is divided by (-IE) is obtained that when $n \to \infty$, then (4) $(E_J)_{n \to \infty} \to 0$ –IE = -IE. This fact is consistent with Zon Equation (1) and $(z_{CT})_{n \to \infty} \to 0$ and therefore electron has jumped all IE and is free from nucleus interaction.

Referenced energy to IE on Y-axis is used in **Figure 8** and n is maintained in X-axis. Curves overlap is also produced in atoms not included in Figure 7 (O and Fe) and, in any case, appreciable deviations are produced in first two Fe jumps. Deviation explanation or possible jumps are not the subject of this introduction.



Figure 9 represents Absolute change for Li, Be, B and C. Actual change vs. n curves have similar morphology and Actual change increases with Z. This situation has happened before with Li and O in previous point (Figures 3 and 5) and, likewise, relationship turns when representation is: % Relative Change (6) vs. n (**Figure 10**). % Relative Change (or %RC) for atoms of second period [Li,Ne] decreases as Z increases until becomes negative %RC. This tendency is conserved for later atoms. Two additional notes: Li is the only that does not meet trend of Figure 10 and some data in higher n have been obviated.

%RC is really low and for atoms of second period [Li,Ne] is located in: [-0,02%,+0,04%]



Once verified that Torrebotana Central Energetic Line (E_J) (4) meets:

- a) Predicts energetic line to which energies of excited states are attracted
- b) This attraction is increased when n and l increase.

c) Same tendencies have been corroborated when atoms, initial configuration and excited state destiny have been changed.

Next step is inclusion of LAN factor in Torrebotana Central Energetic Line (4). LAN creates secondary lines around main or ideal line: Torrebotana Central.

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Abbreviations Table			
Abbreviation	Meaning		
AC	Actual Change		
BES	Born Electronic System		
Ed	Excited state destiny energy		
EJ	Jump energy in Torrebotana Central Line		
E _{J, R}	Referenced E _J to IE		
E_k	Reference Jump energy		
$E_{k, R}$	Referenced E _k to IE		
Eo	1s OES Ionization energy		
El	Es, Ep, Ed and Ef are energies to reach ns, np, nd and nf		

IE	Ionization energy
1	Orbital quantum number
LAN	Serelles Secondary Lines Factor
n	Principal quantum number
NIN	Negative in negative
OES	Origin Electronic System
RC	Relative Change
Z	Effective nuclear charge
Z	Atomic Number
Z _{CT}	Excited state charge
Zo	1s Origin charge according to P46
Zs	Start charge according to P46

ANNEX

Table 5 - Be from $1s^2$ (Term 1S ; J=0) to $1snx$: Actual Change (E _J - E _k)							
Destiny state	1sns	1snp	1snd	1snf			
Term J	¹ S 0	${}^{1}P^{0} 1$	¹ D 2	${}^{1}F^{0}$ 3			
n	Ej-Es	Ej-Ep	Ej-Ed	Ej-Ef			
2	1,62892317	-0,38897683					
3	0,47118696	-0,10971304	0,00538696				
4	0,18802929	-0,03827071	0,00332929	0,00092929			
5		-0,01836997	-0,00666997	0,00053003			
6		-0,01395476		0,00044524			
7		-0,00452239					

Table 6 - Be from $1s^2$ (Term ¹ S; J=0) to 1snx: %RC $100^{(E_J - E_k)/(-IE)}$						
Destiny state	1sns	1snp	1snd	1snf		
Term J	¹ S 0	${}^{1}P^{0} 1$	¹ D 2	${}^{1}F^{0}$ 3		
n	DRP Es (%)	DRP Ep (%)	DRP Ed (%)	DRP Ef (%)		
2	1,05845576	-0,25275273				
3	0,30617193	-0,07129028	0,00350039			
4	0,1221793	-0,02486787	0,00216334	0,00060384		

5	-0,0119366	-0,00433407	0,00034441
6	-0,00906764		0,00028931
7	-0,0029386		

Table 7 - E_k , E_j and z_{CT} for $1s^2$ O till n=8							
n	ZCT	Ej	Es	Ep	Ed	Ef	
2	1,53125	572,533498	568,88661	573,94777			
3	0,68055556	665,196438	664,11143	665,61536	665,23349		
4	0,3828125	697,628467	697,17554	697,79546	697,61816		
5	0,245	712,639863		712,71696	712,68968		
6	0,17013889	720,794202			720,80445		
7	0,125	725,711011					
8	0,09570313	728,902209					

Table 8 - O from $1s^2$ (Term ¹ S; J=0) to 1snx: Actual Change (E _J - E _k)							
Destiny State	1s ¹ ns	1s ¹ np	$1s^{1}nd$	1s ¹ nf			
Term J	${}^{1}S 0$	${}^{1}P^{0} 1$	¹ D 2	¹ F ⁰ 3			
n	Ej-Es	Ej-Ep	Ej-Ed	Ej-Ef			
2	3,6468884	-1,4142716					
3	1,08500818	-0,41892182	-0,03705182				
4	0,4529271	-0,1669929	0,0103071				
5		-0,07709666	-0,04981666				
6			-0,01024796				

Table 9 - O from $1s^2$ (Term ¹ S; J=0) to $1snx: %RC 100*(E_J - E_k)/(-IE)$						
Destiny State	1s ¹ ns	1s ¹ np	1s ¹ nd	1s ¹ nf		
Term J	¹ S 0	${}^{1}P^{0} 1$	¹ D 2	${}^{1}F^{0}$ 3		
n	DRP Es (%)	DRP Ep (%)	DRP Ed (%)	DRP Ef (%)		
2	0,49327151	-0,191292				
3	0,14675624	-0,056663	-0,005012			
4	0,0612621	-0,022587	0,0013941			

5	-0,010428	-0,006738	
6		-0,001386	

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