ARTICLE 13 Relation of Flui Piep de Garberí: LAN⁻¹ and Ionízation Energy. Javier Silvestre <u>www.eeatom.blogspot.com</u>

ABSTRACT

This is 13th article of 24 dedicated to atomic model based on Victoria equation (Articles index is at end). Electon excited states arise around Torrebotana Central Line [1] by Tete-Vic equation which is attached in P47. Serelles Secondary Lines are originated from Torrebotana Central Line by LAN inclusion. Attraction towards Torrebotana Central Line is accentuated as n and l are increased [1,3].

Relation of Flui Piep de Garberí states linear behaviour between inverse of factor seen in Serelles Secondary Line, i.e. LAN, and z_s (Start charge according to P46 non-excited electronic extreme charge). This relation is Z function (atomicity relation) and is connected to P44 Necessary NIN relationships [5] because includes LAN: charge and energy of BES and 1s OES.

Ionization energy (IE) of higher atomic number is estimated from Relation of Flui Piep de Garberí and estimate deviation is grouped according to electron configuration.

KEYWORDS - REVISAR

Relation of Flui Piep de Garberí, Flui Group, IE_{FLUI}, Tete-Vic equation, LAN.

INTRODUCTION

Serelles Secondary Line creation from Torrebotana Central Line is allowed by LAN. Excited states run through Serelles Secondary Lines originating from quantum numbers. LAN(P50) is defined as start or initial LAN of non-excited electron in P50 Initial LAN value in jump from ns to ns. [1,3] This article is focused precisely on non-excited LAN and its relation with z_s and excited state is obviated. z_s is Start charge according to P46 non-excited electronic extreme charge. Abbreviations Table is at end article.

Ionization energy (IE) of higher atomic number can be estimated from Relation of Flui Piep de Garberí once relation between LAN and z_s is established.

P51 Relation of Flui Piep de Garberí

Relation of Flui Piep de Garberí is LAN_s^{-1} vs z_s linearity where suffix s means "start or state non-excited".

 LAN_s equation (1) is the same as that used with LAN(P50), but scope differs:

- P50 Initial LAN value is used in jump from ns to ns because LAN(P50) meets linearity of Relation of Riquelme de Gozy.

- P51 Relation of Flui Piep de Garberí is different from Riquelme de Gozy and $LAN_{\rm s}$ is used for any electron configuration

(1) - LAN_s =
$$\frac{(-E_o)^{1/2} z_s}{(-IE)^{1/2} z_o} - n_{initial}$$

 E_o and z_o are ionization energy and charge of origin electronic system (OES) in all atom: 1s. On the other hand, IE and z_s are referred to ionization energy and charge of start or born electronic system (BES), i.e. electron that is going to be excited. Ionization energy is in [4] and charge is known by P46 non-excited electronic extreme charge [1]. Finally, $n_{initial}$ is n of non-excited electron. (1) is indicated more specifically by (2) where LAN is calculated for electron whose configuration is in parentheses:

(2) - LAN_s(electron configurat ion) =
$$\frac{(-E_o)^{1/2} z_s}{(-IE)^{1/2} z_o} - n_{\text{initial}}$$

2p N LAN_s (therefore, Nitrogen has already lost 2 electrons) is expressed in (3):

(3)LAN_s(2p N) =
$$-\left(\frac{(667,04609 \text{ eV})^{1/2}3}{(47,4453 \text{ eV})^{1/2}7} - 2\right) = 0,393042 \text{ Lanitos}$$

LAN and LAN⁻¹ for 2s BES with z_s =[1-10] is in **Table 1**. Figure 1 is representation of Flui Piep de Garberí: LAN_s⁻¹ vs z_s . Linear regression is very good with R²=1,0000. Lanito is LAN unit although LAN is added to n that lacks unit [2,3]. Representation can be performed in any unit advancement mode because z_s progresses one by one (P46). Figure 1.B. is as Figure 1, but with atomic symbol on X-axis.

	Table 1 - LAN and LAN ⁻¹ for 2s with $z_s=[1-10]$								
Symbol	Z_{2s}	LAN (n=2) (Lanito)	LAN ⁻¹ (n=2) (Lanito) ⁻¹						
Li	1	0,41144445	2,43046176						
Be	2	0,27118299	3,68754687						
В	3	0,20303233	4,92532393						
С	4	0,16242214	6,15679624						
Ν	5	0,13542253	7,38429585						
0	6	0,11615164	8,60943468						
F	7	0,10171511	9,8313808						
Ne	8	0,09048397	11,0516815						
Na	9	0,08151353	12,2679027						
Mg	10	0,07419118	13,4786909						



Relation of Flui Piep de Garberí (4) is calculated for rest of electron configurations in n=2 and also are obtained linear tendencies whose line equations and R^2 are shown in **Table 2** and **Figure 2**. Linear tendencies are made with first 10 atoms of each configuration as in Figure 1.

Table 2 - Line equations of Flui Piep de Garberí for electron configurationsin n=2 (made with first 10 atoms)									
System	a (lanito) ⁻¹	b (lanito) ⁻¹	\mathbb{R}^2						
28	1,23644	1,22653	1,0000						
$2s^2$	0,70203	0,59407	0,9999						
2p	0,87225	0,55313	0,9999						
2p ²	0,72920	0,41100	0,9999						
2p ³	0,66550	0,32825	0,9999						
2p ⁴	0,72939	0,29936	0,9998						
2p ⁵	0,66675	0,25567	0,9998						
2p ⁶	0,63703	0,22102	0,9996						



Figure 3 shows linear trend of Figure 1 by "2s". In addition, 2s Ionization Energy (IE in (2)) increases are included in "2s mod." where "mod." is modified abbreviation. IE changes are realized on atoms with 2s charge=3, 6 and 9 which are corresponding to B, O and Na according to P46 [1]. Increase is equal to 0,25% IE and its effect is more noticeable as z_s is longer.

$$(4) \frac{1}{LAN_s} = a + bz_s$$



2s IE in atoms after Mg (last in Table 1) are calculated from Relation of Flui Piep de Garberí (4) and compared with reference [4] to verify linear trend evolution. (4) is transformed into (5) by (2) inclusion. 1s Ionization Energy (E_0) is provided by [4]. IE_{FLUI} is IE estimated with Relation of Flui Piep de Garberí.

(5) LAN_{FLUI} =
$$-\left(\frac{(-E_o)^{1/2} z_s}{(-IE_{FLUI})^{1/2} z_o} - n_{initial}\right) = \frac{1}{a + bz_s}$$

IE is obtained in (6) from (5):

(6) IE_{FLUI} =
$$-\left(\frac{-(-E_o)^{1/2} z_s(a+bz_s)}{z_o(1-n_s(a+bz_s))}\right)^2 = -\left(\frac{-(-E_o)^{1/2} z_s}{(LAN_{FLUI}-n)z_o}\right)^2$$

Table 3 compiles E_o , as well as 1s OES charge (z_o) and 2s charge (z_s). LAN⁻¹ is calculated from Relation of Flui Piep de Garberí (4) with line equation (Table 2). IE_R and IE_{FLUI} (6) are Ionization Energy with reference [4] and calculated by equation (6) respectively for comparison in last two table columns. Suffix R means "Reference" and "FLUI" indicates that has been obtained by Relation of Flui Piep de Garberí. (7) is actual change (AC) and Relative Change in percentage for IE estimated is given in (8):

(7) Actual Change (IE) =
$$AC(IE) = \Delta = IE_{FLUI} - IE_R$$

(8)%RC(IE) = $\frac{(IE_{FLUI} - IE_R)}{/IE_R/} *100$

	Tabla 3 - IE _{FLUI} estimated for 2s ($z_s>10$)								
Atom	E _o (eV)	Zo	Zs	LAN ⁻¹ (lanito ⁻¹)	$IE_{R} (eV)$	IE _{FLUI} (6) (eV)	AC (eV)	% RC	
Al	-2304,141	13	11	14,72827	-442	-441,923	0,07659	0,017%	
Si	-2673,182	14	12	15,9548	-523,42	-523,276	0,14389	0,027%	
Р	-3069,842	15	13	17,18133	-611,74	-611,522	0,21752	0,036%	
S	-3494,1892	16	14	18,40786	-707,01	-706,678	0,33170	0,047%	
Cl	-3946,296	17	15	19,63439	-809,4	-808,760	0,63951	0,079%	
Ar	-4426,2296	18	16	20,86092	-918,03	-917,785	0,24486	0,027%	
K	-4934,046	19	17	22,08745	-1033,4	-1033,766	-0,36616	-0,035%	
Ca	-5469,864	20	18	23,31398	-1157,8	-1156,731	1,06925	0,092%	
Sc	-6033,754	21	19	24,54051	-1287,956	-1286,696	1,25975	0,098%	
Ti	-6625,807	22	20	25,76704	-1425,257	-1423,684	1,57253	0,110%	
V	-7246,1223	23	21	26,99357	-1569,656	-1567,719	1,93683	0,123%	
Cr	-7894,7989	24	22	28,2201	-1721,183	-1718,824	2,35876	0,137%	
Mn	-8571,9485	25	23	29,44663	-1879,873	-1877,026	2,84654	0,151%	
Fe	-9277,6814	26	24	30,67316	-2045,759	-2042,352	3,40651	0,167%	
Со	-10012,122	27	25	31,89969	-2218,876	-2214,832	4,04377	0,182%	
Ni	-10775,386	28	26	33,12622	-2399,259	-2394,494	4,76517	0,199%	
Cu	-11567,612	29	27	34,35275	-2586,954	-2581,371	5,58337	0,216%	
Zn	-12388,928	30	28	35,57928	-2781,996	-2775,494	6,50221	0,234%	
Ga	-13239,488	31	29	36,80581	-2984,426	-2976,900	7,52559	0,252%	
Ge	-14119,429	32	30	38,03234	-3194,293	-3185,624	8,66907	0,271%	
As	-15028,906	33	31	39,25887	-3411,643	-3401,702	9,94103	0,291%	
Se	-15968,083	34	32	40,4854	-3636,526	-3625,174	11,35171	0,312%	
Br	-16937,126	35	33	41,71193	-3868,986	-3856,081	12,90471	0,334%	
Kr	-17936,208	36	34	42,93846	-4109,083	-4094,465	14,61794	0,356%	
Xe	-41299,71	54	52	65,016	-9810,4	-9723,258	87,14209	0,888%	

 $\rm IE_{FLUI}$ maintains correct correlation with $\rm IE_R$ and Relative Change (8) is less than 0,1% after 9 estimated atoms. In addition, differences fulfil continuous ascent that is corroborated after jump to atoms of greater zs as Xenon and Lutetium.

Lu	-73804,8	71	69	85,86701	-17928,05	17631,069	296,9811	1,657%
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Relation of Flui Piep de Garberí (4) for n=3 is in **Figure 4** with atoms between Na and Fe in X-axis. Main conclusion is that linear trends are maintained when n=3.



P52 IE deviation tendency in Relation of Flui Piep de Garberí

IE deviation between ionization energy by Flui Piep de Garberí (6) and reference [4] is not random and its tendency is function of electron configuration and energy. Variation increases with atomic number and is consequently correlated with P44 Necessary NIN relationships [5] where is indicated: "Probability factors included in lobe or Electronic System have tendencies that are fulfilled through electronic extreme charge."

Procedure is:

A) IE_{FLUI} or Ionization energy by (6) is calculated up to Z=100 (Fm) with line equations of Flui Piep de Garberí for electron configurations in n=2 (made with first 10 atoms). Ionization energy (IE_R) reference is in [4]

B) Actual Change is obtained by (7).

C) Deviation for 1s is given by (9) where 1s theoretical ionization energy is E_{oT} and E_o is 1s reference ionization energy.

$$(9)AC(1s IE) = E_{oT} - E_o = -13,6056899Z^2 - E_o$$

D) $1s^2$ Actual Change (7) is added to study. As in n=2, first 10 atoms are used for linear regression in LAN⁻¹ vs. z_s representation. Linear trend is excellent: $R^2=1,00000$ and its equation is: LAN⁻¹(1s²) = 1,21244 + 2,68298 z_s (**Figure 5**)

Once Relation of Flui Piep de Garberí (4) is known, IE_{FLUI} is calculated (6) and its Actual Change (7).



E) Actual Change of IE or AC(IE) (7) vs IE_R are made in Figure 6 (1:1 scale) and Figure 7 (Y axis is reduced to better contemplate trends).

Observations in Figure 6 and 7:

E.1) Actual Change of Ionization Energy (AC (IE)) in n=1

Actual Change (7) for 1s in absolute value is much greater than for $1s^2$:

$$/AC (1s IE) / >> /AC (1s^{2} IE) /$$

For example, Relative Change in percentage for IE (8) when IE=-40000 eV is:

$$/\%$$
 RC (1s IE)/ $\approx 4 \% >> /\%$ RC (1s² IE)/ $\approx 0.18 \%$

In fact, Germanium must be reached so that there is % $RC(1s^2 \text{ Ge IE}) \approx 0.1\%$ with IE_R=-13557,4202 eV and IE_{FLUI}= -13570,4807 eV.



E.2) Actual Change of Ionization Energy (AC (IE)) in n=2

Actual Change in n=2 can be subdivided into two Flui groups:

* Flui Group I is 2s, $2s^2$, 2p and $2p^2$: AC (IE) vs. IE_R curves have same sign and similar morphology and values as 1s curve.

* Flui Group II is from $2p^3$ to $2p^6$ and has sign opposite to Group I AC (IE) and with greater absolute value without this avoiding that their curves are almost overlapping.

As consequence of these near-overlapping, **Table 4** can be made with approximate values of % RC (IE) as IE function for these two groups and $1s^2$. It must be considered that high Atomic Number (Z>40) is required for reach /IE/ > 5000 eV in n=2.

% RC (IE) for IE \approx -2000 eV in n=2 that already implies to be on Z \approx [26,30] is:

	Table 4 - Relative Change in percentage for IE (8) in n=1 and 2										
	Energía (eV)										
	Electron Configuration	2000	5000	10000	15000	20000	25000	30000	35000		
IE)	Group I and 1s	-0,1	-0,5	-0,8	-1,1	-1,5	-2	-2,5	-3,3		
RC (Group II	0,2-1,0	1,5	4	6	8	12	14			
%]	$1s^2$	-0,01	-0,05	-0,08	-0,10	-0,12	-0,14	-0,15	-0,17		

E.3) Actual Change of Ionization Energy (AC (IE)) in n=3

Actual Change of Ionization Energy in n=3 or AC (n=3 IE) can be subdivided into four groups and the first two groups correspond to those seen in n=2. Groups are summarized in **Table 5** for n>1. Flui Groups are separated by semi-full orbital (np³, nd⁵, nf⁷...)

Table 5 -Groups Flui according to behaviour withP44 Necessary NIN relationships [5]						
Flui Group	Electron configuration					
Ι	From ns to np ²					
Π	From np ³ to np ⁶					
III	From nd to nd ⁴					
IV	From nd ⁵ to nd ¹⁰					
V	From nf to nf ⁶					
VI	From nf ⁷ to nf ¹⁴					

Figure 8 is AC (n=3 IE) vs IE_R representation:

* Same grouping trends and morphology curves seen with n=2

* AC (n=3 IE) of four Flui groups is negative as opposed to those seen in AC (n=2 IE) of Flui Group I (from 2s to $2p^2$ and 1s) whose value is positive (Figure 6 and 7)





* Generally and for Flui Group higher than I, following inequality is fulfilled when representation is AC (IE) vs IE_R :

(10) /AC (n=3 IE)/ >/AC (n=2 IE)/ in AC (IE) vs IE_R representation and Group>I

This fact is best seen in **Figure 9** where $2p^6$ and $3p^6$ are represented.

* In contrast (10) inequality is modified if representation is AC (IE) vs E_0 (Figure 10) where E_0 is 1s ionization energy (11):

(11) /AC (n=3 IE)/ < /AC (n=2 IE)/ in AC (IE) vs E_o representation and Group>I



LAN covers both energies and its Actual Change is studied in following point.

P53 Flui LAN Equilibrium: LAN deviation in Relation of Flui Piep de Garberí

Actual Change (LAN) vs. $E_{\rm o}$ curves of different Flui Groups are annulated with each other.

Actual Change of LAN or AC (LAN) (12) is given by equation analogous to Actual Change (IE) (7):

(12) Actual Change (LAN) = $AC(LAN) = \Delta = LAN_{FLUI} - LAN_R$

AC (LAN) vs. E_o behaviours that deserve to be highlighted:

A) Linearity versus curvature of previous representation (AC (IE) vs. IE_R: or E_o)

Actual Change (LAN) of $2p^4$ and $3p^4$ vs. E_0 trace high linearity with R²=0.9998 (Figure 11). Both lines have initial short bending curve ($2p^4$ C and $3p^4$ C where C indicates Curve). Curvature region grows as n increases (Figure 11.B. includes $4p^4$).



At this moment, electron configuration applied should be commented on because $4p^4$ has been represented. As z_s represented is high, selected configuration is that corresponding to progressive closure of n quantum numbers. This selected configuration is supported by reference [4]. For example, consecutive order for 78 Pu XVI electrons is (13):

(13)
$$1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4s^2 4p^6 4d^{10} 4f^{14} 5s^2 5p^6 5d^{10}$$

Consecutive order is not the one indicated by Periodic Table (14):

(14)
$$1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^{10} 4p^6 5s^2 4d^{10} 5p^6 6s^2 4f^{14} 5d^8$$

Extended consecutive order is given by (15) and is applied throughout article:

(15) $1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4s^2 4p^6 4d^{10} 4f^{14} 5s^2 5p^6 5d^{10} 5f^{14} 5g^{18} 6s^2 6p^6 6d^{10} 6f^{14} 6g^{18}...$

B) Flui Groups are maintained in AC (LAN) vs Eo

An example is Flui Groups in n=2 represented in Figure 12.



C) Flui Equilibrium (FE)

C.1) Flui Equilibrium in n=2 or FE(n=2)

Simple arithmetic operations with Flui Groups are performed to nullify AC (LAN). Flui Equilibrium in n=2 is calculated by (16). For example, sum of AC(LAN) from $2p^3$ to $2p^6$ (Flui Group II) in n=2 is abbreviated as \sum FGII(n = 2). 4 Flui Groups of FGI are divided by 4 and \sum FGII(n = 2) only counts as one single FGI, i.e. $\frac{1}{4}\sum$ FGI(n = 2), and is consequently divided by 4*4. Figure 13 represents FE(n=2) (Flui Equilibrium in n=2) where AC(LAN) cancellation is observed.

$$(16)FE(n=2) = \frac{\sum FGI(n=2)}{4} + \frac{1}{4} \frac{\sum FGII(n=2)}{4} = \frac{\sum FGI(n=2)}{4} + \frac{\sum FGII(n=2)}{16}$$

Direct Sum provides by configuration (17) provides good result even thought annulment is slightly smaller:



$$(17)FE(2s^{2}2p^{6}) = AC(2s^{2}LAN) + \frac{AC(2p^{6}LAN)}{4}$$

C.2) Flui Equilibrium in n=3 or FE(n=3)

Situation is more complicated in n=3 and first problem is that all AC(n=3) are positive as $/E_o/$ increases. AC(LAN) arithmetic mean of electron configuration of each Flui Group (Table 5) is represented in **Figure 14**. Electron configurations from each Flui Group maintain overlap in AC(LAN) vs E_o seen in previous point (**Figure 12**).



This first problem conceives two possible solutions proposed:

* Arithmetic operations must include negative signs prior to summations.

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* AC(LAN) cancellation is achieved because AC(LAN) in n=3 is, like AC(LAN) of Group II in n=2 (Figure 13), neutralized with AC(LAN) of Group I in n=2 that has negative sign. (16) can be transformed into (18) for n=3. Explanation for fractions follows (18):

$$(18)FE(n=3) = \frac{\sum FGI(n=2)}{4} + \frac{\sum_{i=1}^{N} FG_i(n=3)}{4} = \frac{\sum FGI(n=2)}{4} + \frac{1}{4} \frac{1}{3} \left(\frac{\sum FGI(n=3)}{4} + \frac{\sum FGII(n=3)}{4} + \frac{\sum FGII(n=3)}{4} + \frac{1}{2} \left(\frac{\sum FGIII(n=3)}{4} + \frac{\sum FGIV(n=3)}{6} \right) \right)$$

Comments of fractions included in (18):

$$\frac{\sum FGI(n=2)}{4}$$
 4 electron configuration: From 2s to 2p²
+ $\frac{1}{4}$ (FG(n=3) sum) As in previous case in n=2, all Groups other than Group I only counts as one single FGI

 $\frac{1}{3}$ (FG(n = 3) sum) There are 3 summands: FGI, FGII and d configuration (subdivided into 2 groups: FGIII and FGIV)

 $\frac{\sum FGIV(n=3)}{6}$ Fraction is number of electron configuration. For example, 6 are in FGIV (From nd⁵ to nd¹⁰).

$$\frac{1}{2} \left(\frac{\sum FGIII(n=3)}{4} + \frac{\sum FGIV(n=3)}{6} \right)$$
 2 is because d configuration is subdivided
into 2 groups: FGIII and FGIV

As in the previous point, direct Sum provides by configuration (19) provides good result and its annulment result is only slightly lower than (18). Trend is correct and is directed towards nullification as $-E_0$ increases.

$$(19)FE(3s^{2}3p^{6}3d^{10}) = AC(2s^{2} LAN) + \frac{1}{4}\frac{1}{3}(AC(3s^{2} LAN) + AC(3p^{6} LAN) + AC(3d^{10} LAN))$$



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Abbreviations Table

Following Table indicates abbreviations used in this theory and its use in article in question is marked with X. 10, 11 and 12 are [1] [2] and [3] respectively. 13 is present article.

Abbreviation	10	11	12	13	Meaning
AC	Х		Х	Х	Actual Change
BES	Х	Х		Х	Born Electronic System
Ed	Х	Х			Excited state destiny energy
E _{dA}			Х		Destiny Energy deduced with Xorrador Approximation
EdI		Х			Excited state destiny energy obtained from ideal E_d
E _{dR}		Х	Х		Reference destiny energy
E_{dRI}		X	X		Ideal E_{dR} obtained from extrapolation of others E_{dR} satisfying Relation of Riquelme de Gozy
Eds		Х			Excited state destiny energy in Serelles Secondary Line
EJ	Х	Х			Jump energy in Torrebotana Central Line
EJA			Х		Jump Energy deduced with Xorrador Approximation
E _{J, R}	Х				Referenced E _J to IE
EJS		Χ			Jump energy in Serelles Secondary Line
E _k	Х	Х	Х		Reference Jump energy
E _{k, R}	Х				Referenced E _k to IE
Eo	Х	Х	Х	Х	1s OES Ionization energy
E _{oT}				Х	1s theoretical ionization energy
FE				Х	Flui Equilibrium
FG				Х	Flui Group
El	Х	Х			Es, Ep, Ed and Ef are energies to reach ns, np, nd & nf
IE	Х	Х	Х	Х	Ionization energy
IE _{FLUI}				Х	IE estimated with Relation of Flui Piep de Garberí
1	Х	Х	Х	Х	Orbital quantum number
LAN	Х	Х	Х	Х	Serelles Secondary Lines Factor
LAN _I LAN _{RI}		Х			Ideal LAN obtained from E _d or E _{dRI}
LAN _R		Х	Х		LAN with reference data
LAN _{R,M}		Х			LAN _R with modification
LANs				Х	LAN(P50) used for any electron configuration

LAN(P50)		Χ	Χ	Χ	Initial LAN value in ns to ns jump. LAN with IE
n	Χ	Χ	Χ	Χ	Principal quantum number
n _{initial} or n _s		Х	Χ	Χ	n of non-excited electron
NIN	Χ			Χ	Negative in negative
OES	Χ	Χ		Χ	Origin Electronic System
RC	Χ		Χ	Χ	Relative Change
Z	Χ				Effective nuclear charge
Z	Χ			Χ	Atomic Number
ZCT	Χ	Х			Excited state charge
Zo	Χ	Х	Χ	Χ	1s Origin charge according to P46
Zs	Χ	Х	Χ	Χ	Start charge according to P46
Z _{SS}		Χ			Serelles secondary charge

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