

## ARTICLE 08

### ELECTRON PROBABILITY WITH NIN COUPLING IN $n=2$

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#### ABSTRACT

This is 8th article of 24 dedicated to atomic model based on Victoria equation (Articles index is at end). A and B Electronic Extremes Probability ( $P_i$ ) curves with Geometric NIN Coupling (GNC) and Probabilistic NIN Coupling (PNC) are studied in  $n=2$  quantum number.  $C_{PEP}$ ,  $C_{POTI}$  and  $z$  data [7] are used.  $H_i$  vs.  $c_i$  is represented in GNC and  $P_i$  vs.  $r_i$  in PNC. Maximum  $P_i$  is calculated with  $r_i$  variation of 0,1 pm and compared with references. Finally, by way of example, Nitrogen outermost electron is represented both when reaches  $C_{POTI}$  angular limit ( $C_{POTI-AL}$ ) and for lobe always growing (LAG) [5].

#### KEYWORDS

NIN coupling in  $n=2$ , Electron Probability, Maximum Probability, OES, BES, OPA jump, Victoria Equation.

#### INTRODUCTION

This is 8<sup>th</sup> article of 24 dedicated to atomic model based on Victoria equation (Articles index is at end). A extern electronic extreme ( $EE_A$ ) is indicated with a suffix ( $r_A$ ,  $H_A$  or  $c_A$ ), B intern with b suffix ( $r_B$ ,  $h_B$  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 [6,7], at article end.

A and B are  $EE_i$  introduced with Victoria Equation [1]. Geometry is based on right-angled triangle where sides are  $r_i$ ,  $H_i$  and  $c_i$  [2].  $P_i$  concept is closely related to  $c_i$  and electron energy ( $E_i$ ) [3].  $c_i$  compaction and  $P_i$  coupling between lobes in the same  $n$  are studied [3,7]. Maximum  $P_i$  is visually approximated for  $2p^5$  Fluorine example [6]. GNC, PNC and maximum  $P_i$  are analyzed in more detail with method with  $r_i$  defined and  $C_{PEP}=1$  for Oxygen lobes in  $n=2$  [7].

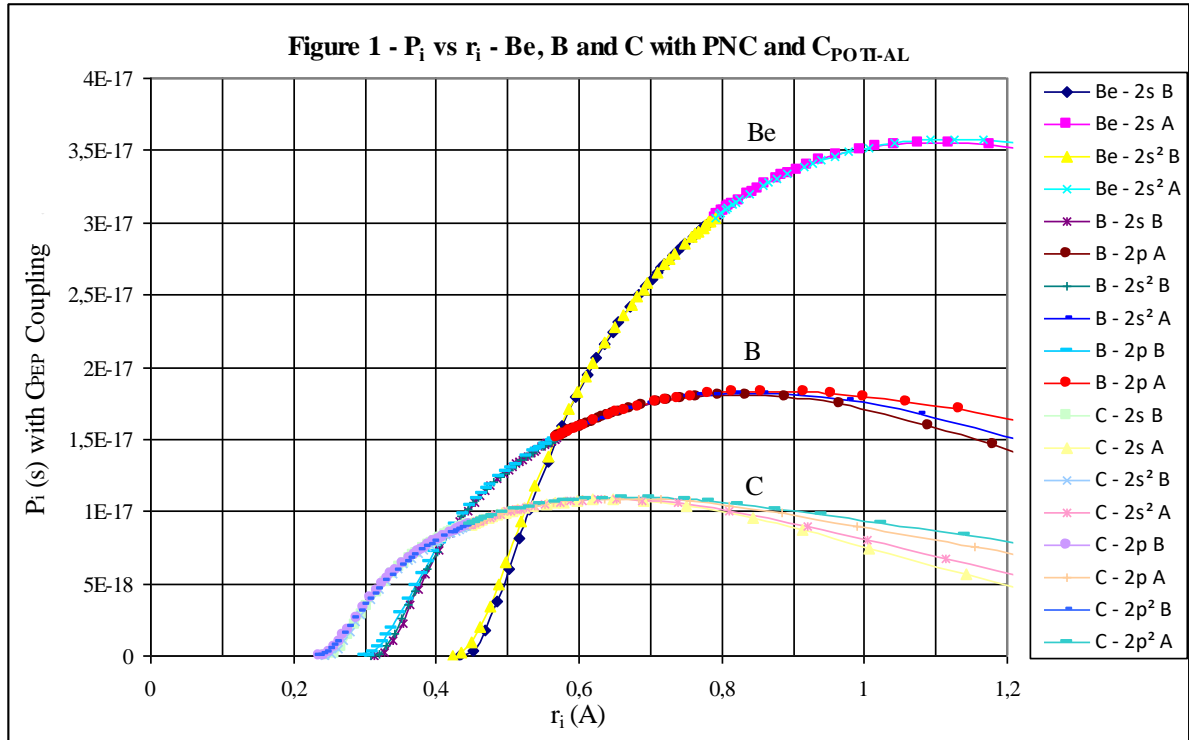
After these previous points, geometric and probabilistic study is extended to all atoms whose last shell is  $n=2$  (from Li to Ne).

#### $P_i$ curves for atoms in $n=2$

Following figures have been made applying:

- 1) Victoria Equation for energy radial distribution [1]
- 2)  $r_i$ ,  $c_i$  and  $H_i$  relation [2]
- 3)  $c_i$  and  $P_i$  with Compaction Factor ( $C_F$ ) and Three Feliz Solutions [3,5]
- 4) Feliz IV:  $P_i$  curves with NIN coupling in  $n$  quantum number [6,7]

$P_i$  vs.  $r_i$  or Probability radial distribution is shown for Be, B and C in  $n=2$  (**Figure 1**). Figure 1 is PNC representation since, in addition to considering  $z$ , MON and  $C_{\text{POTI-AL}}$  couplings, includes  $C_{\text{PEP}}$ .



In Figure 1 can be verified:

a) 2s Origin Electronic System (OES) and all Born Electronic System (BES) are represented fulfilling PNC as has been made with Oxygen [7].

b)  $P_i$  curves deepen towards nucleus as atomic number increases in all OES. This effect can be predicted if is considered as seen in [1] that both  $r_B$  when its division tends to 0 ( $r_B$ ) $_{d \rightarrow 0}$  and two  $EE_i$  when its division tends to infinite ( $r_i$ ) $_{d \rightarrow \infty}$  are proportional to  $-z/E_o$ .  $E_o$  is initial energy and is Ionization Energy (IE) whenever electron is in ground state (P03 [1]) and  $z$  is Effective nuclear charge on electron (P14 [1] and P41 [6]).

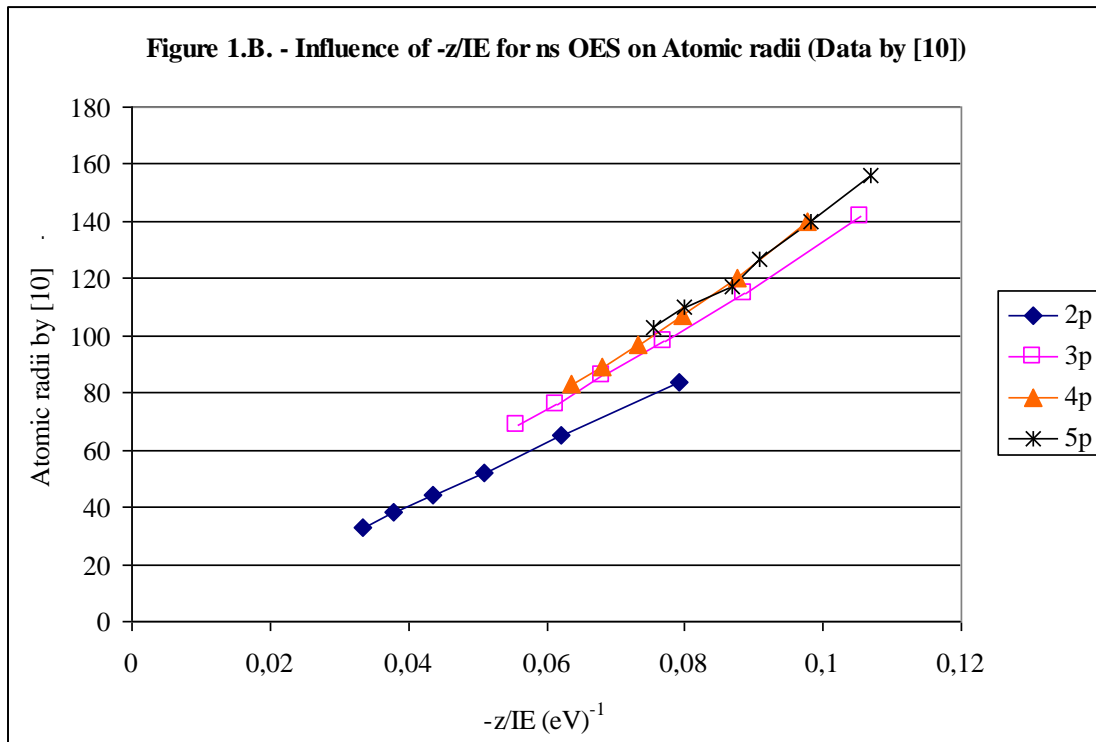
OES is governed by P14 and  $z=Z-2$  where  $Z=$  Atomic number.  $-z/IE$  ratio decreases as atomic number increases (**Table 1**) and, therefore, two curve basic points ( $(r_B)_{d \rightarrow 0}$  and  $(r_i)_{d \rightarrow \infty}$ ) are deeper when atomic number is higher.

Symbol	Li	Be	B	C	N
$-z/IE$	0,1854698	0,1098228	0,0790919	0,0620217	0,0510777
Symbol	O	F	Ne	Na	Mg
$-z/IE$	0,0434408	0,0377997	0,0334592	0,0300136	0,0272109

Relation between  $-z/EI$  for ns OES and Maximum Probability (provided by [10]) seems to exist (**Figure 1.B.**). Six points corresponding to 2p-block produce an approximately straight line with an optimal regression coefficient ( $R^2=0.9997$ ) and an ordinate that tends towards origin ("electron with  $-z/EI=0$  for ns OES  $\rightarrow$  Maximum  $P_i=0$ "). Six 2p-block atoms have  $MON=10$  for OES. Remaining p-blocks also present same behaviour as 2p-block although:

- 1) Their points are better adjusted with second degree polynomial trend.
- 2) p-blocks born from 3s, 4s and 5s OES are grouped and somewhat separated from 2p-block. This fact is correlated with OES MON for 3p-block, 4p-block and 5p-block that are close and relatively distant to OES MON for 2p-block (**Table 1.B.**).

np-block	2	3	4	5
OES MON	10	4	3	2



Beyond  $(r_A)_{d \rightarrow \infty}$ ,  $r_A$  has not been commented because there are few differences between these atoms since MON is same or similar (12.5 for Be and 10 from B (P37 and P38 [6]) and consequently in curve morphology.

BES is conformed to these guidelines by being subjected to NIN coupling (P34 [6]) and its radial curves are also more internal as atomic number increases.

c) If all OES has  $C_{PEP}=1$ ,  $P_i$  decreases when atomic number ( $Z$ ), and therefore also  $z$  (P14 [1]), increases. Reason lies in Probability concept [3] that is develop up to (1):

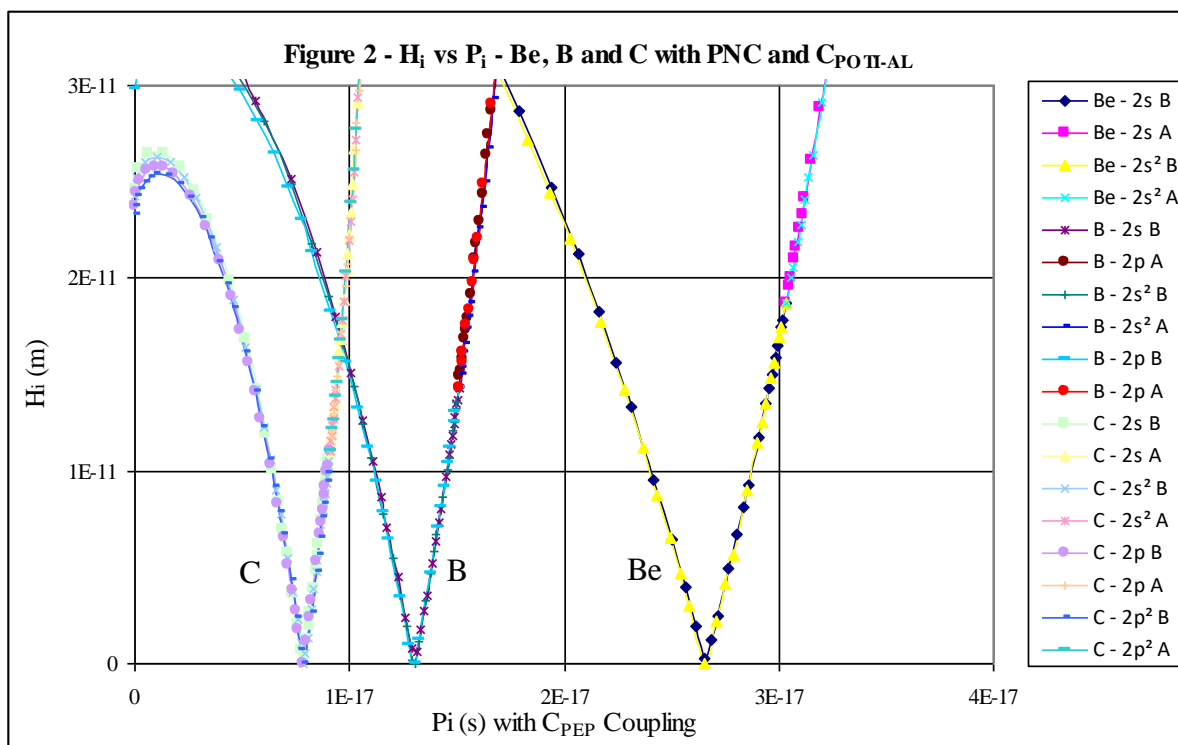
$$(1) P_i = \frac{\hbar}{C_F m_e v_i^2}$$

IE and  $z$  provides higher EE velocity ( $v_i$ ) as  $Z$  increases. As velocity is higher, (1) denominator increases and  $P_i$  is lower. Other parameters have little relevance since  $\hbar$  and  $m_e$  are constants and  $C_F$  is very similar in this case because:

- 1) PEP=2 (P27 [3]).
- 2) 2s OES MON is similar: 12.5 for Be and 10 from B (P37 and P38 [6]).
- 3)  $C_{PEP}=1$  for OES.
- 4)  $C_{POTI}$  is very similar but not the same since representation is made based on  $C_{POTI-AL}$  [6] and values differ slightly [7].

d) Maximum  $P_i$  is in agreement with references [9] and [10]. This point is amplified in second article part.

$H_i$  vs.  $P_i$  is another PNC curve (**Figure 2**) with same atoms (Be, B and C) as in Figure 1. In addition to comments in Figure 1,  $C_{POTI-AL}$  application and its coupling are observed.

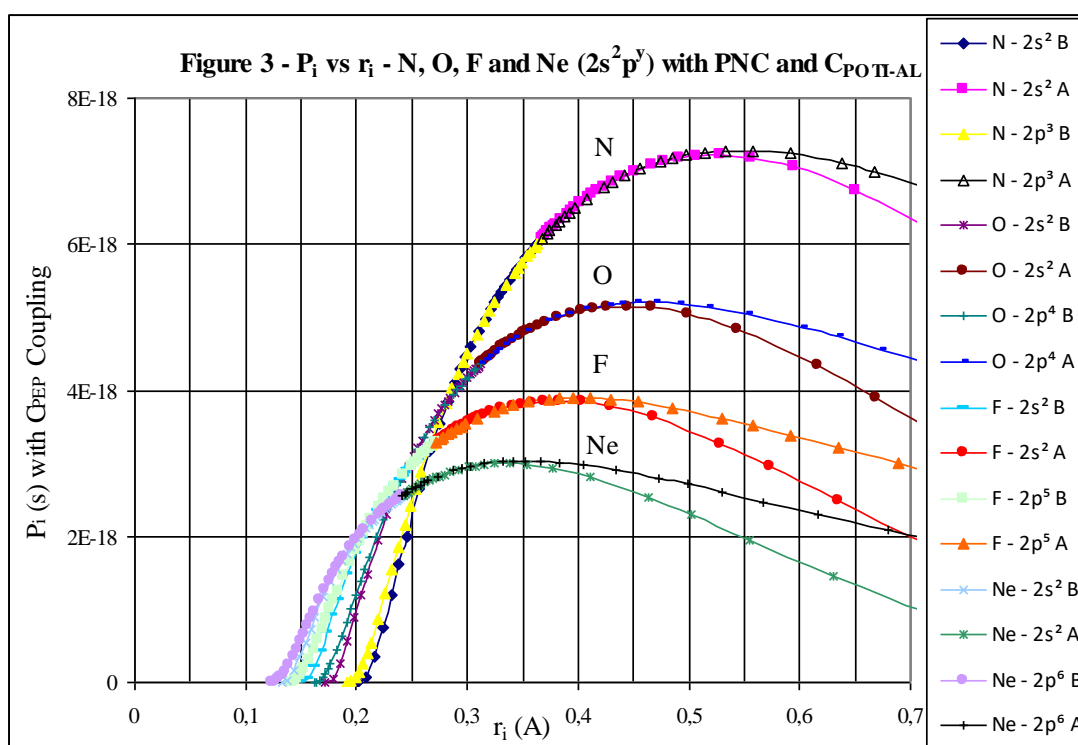


NIN coupling solves an apparent rarity:

- 1) Nitrogen outermost electron energy (-14,53413 eV) is about one electron volt more energetic than Oxygen (-13,618054 eV).
- 2) In principle, electron more energetic should be attracted with more force by nucleus and therefore be more intern.

This relationship between outermost electron IE and maximum electron probability is fulfilled in period, but Oxygen, being less energetic than Nitrogen, has its maximum closer to nucleus (46 and 44 pm for O and 52 pm for N ([9] and [10])).

NIN coupling explanation for this alleged anomaly is that OES is deeper when Z is higher (see b) comment on Figure 1) and outermost lobe together with rest of BES are coupled to OES. In **Figure 3** is represented  $P_i$  vs.  $r_i$  in  $n=2$  for N, O, F and Ne.  $2s^2$  lobe in  $n=2$  and outermost lobe ( $2p^y$ ) have been selected, i.e. theoretical electronic configuration for external shell.



Maximum  $P_i$  radius is lower in O than in N, even with lower -EI of outermost electron, because NIN coupling compensates it with  $z$  ( $z(2p^3 \text{ N})=0.74237$  vs.  $z(2p^4 \text{ O})=0.5918$  [7]) and greater  $z$  for a given IE implies lower interaction nucleus-electron implying electron further away from nucleus.

### Maximum Probability calculation

The most detailed maximum  $P_i$  analysis is carried out in  $EE_A$  which is where maximum is produced. Victoria Equation [1] is performed considering  $r_A$  instead of division ( $d$ ). For this, in Victoria Equation is employed (2) where  $d=f(r_A)$  as has been done in Oxygen example [7]. In this article,  $r_A$  differentials go from 0.5 (Oxygen example) to 0.1 for greater accuracy.

$$(2) d = \frac{E_o \lambda + \frac{F \lambda}{2r_A}}{F + E_o \Gamma_A}$$

Three methods have been applied to predict maximum electronic density probability:

1)  $P_i$  Maximum by extern system.

$P_i$  maximum is given exclusively by maximum of outermost lobe  $P_i$ . In fluorine example [6], this method is used though only visually and based on  $P_i$  vs.  $r_i$  graphical representation. With  $r_i=0,5$  pm variations is employed in  $2s^2$  and  $2p^4$  lobes for Oxygen case [7].

2) Lobes  $P_i$  sum ( $C_{PEP}=1$ )

This method is applied in [7] for Oxygen with  $r_i=0.5$  pm variations and basically is lobes  $P_i$  sum with  $C_{PEP}=1$  in a concrete n.

3) Lobes  $P_i$  sum with  $C_{PEP}$  coupling.

This method is same as above, but considering  $C_{PEP}$  coupling (P42 [6]). Electron extern  $P_i$  is reduced because is referred to OES, so decreases its importance in (3) and Probability weighted average is slightly lower. Probability weighted average in (3) is for  $ns^x np^y$  configuration and is used for methods 2 and 3.

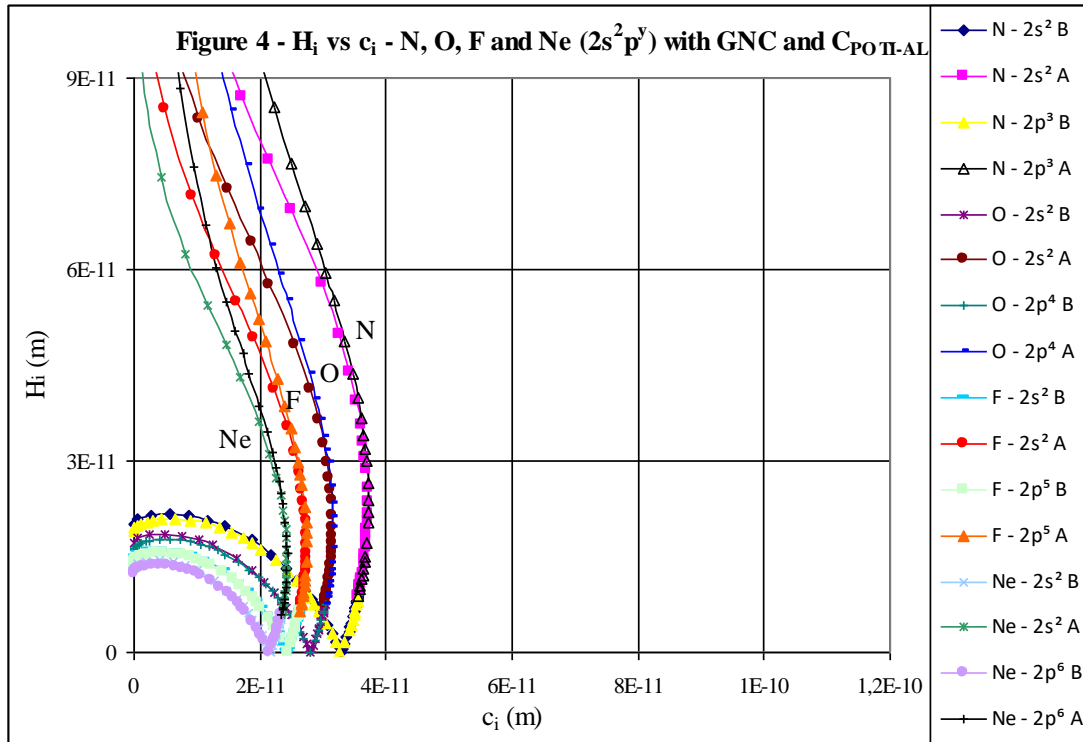
$$(3) (P_i)_{ns^x np^y} = \frac{xP_s + yP_y}{x + y}$$

After lobe individual  $P_i$  calculation with  $r_i=0.5$  pm variations, three methods are applied and maximum  $P_i$  is collected in **Table 2**. Comparative with [9] and [10] are optimal and values obtained with 3 methods are similar.

<b>Table 2 – radius of maximum <math>P_i</math> vs. [9] and [10]</b>				
Atoms	<b>Li</b>	<b>Be</b>	<b>B</b>	<b>C</b>
By extern lobe			86,7	67,0
Lobes $P_i$ sum ( $C_{PEP}=1$ )	162,8	112,3	84,8	65,6
Lobes $P_i$ sum with $C_{PEP}$ coupling			85,1	66,0
[9]	167	111	83	65
[10]	164	108	84	65
Atoms	<b>N</b>	<b>O</b>	<b>F</b>	<b>Ne</b>
By extern lobe	54,7	46,3	40,1	35,3
Lobes $P_i$ sum ( $C_{PEP}=1$ )	53,6	45,5	39,4	34,8
Lobes $P_i$ sum with $C_{PEP}$ coupling	54,1	45,9	39,8	35,1
[9]	52	46	41	Not reported
[10]	52	44	38	33

## Geometric representations

$H_i$  vs  $c_i$  GNC is represented in **Figure 4**. For this NIN coupling is sufficient with  $z$ , MON and  $C_{POTI}$  couplings;  $C_{PEP}$  Coupling is not required [6]. Two axes have been made in 1:1 scale to better evidence geometry.  $s$  and  $p$  lobes are contracted as atomic number increases. Finally, to note that  $s$  lobe shape is indicated to observe curves overlap since its shape is spherical symmetry as is justified in P18 Rotation movement or fixation of Orbital Plans Axis (OPA) [2].



## Nitrogen $2p^3$ orbital representation

$2p^3$  BES data obtained [7] are included in **Table 3**. Lobe flat geometry ( $H_i$  vs.  $c_i$ ) can be represented with this data. Orbital circumference ( $c_i$ ) must know radial distance ( $r_i$ ) [1] and  $C_F$  [3,7]. Circular orbital height ( $H_i$ ) needs to know  $r_i$  and  $h_i$  [2]. Concrete geometry corresponds to  $C_{POTI-AL}$  with  $\alpha_{NOA}=180$  degrees [6] in **Figures 5** and **Figure 6**.

Energy (eV)	PEP	$z$	MON	$C_{POTI-AL}$
-14,53413	2	0.74237	67.35190	1.3931891

Figure 5 -  $2p^3$  Nitrogen with  $C_{POTI-AL}$

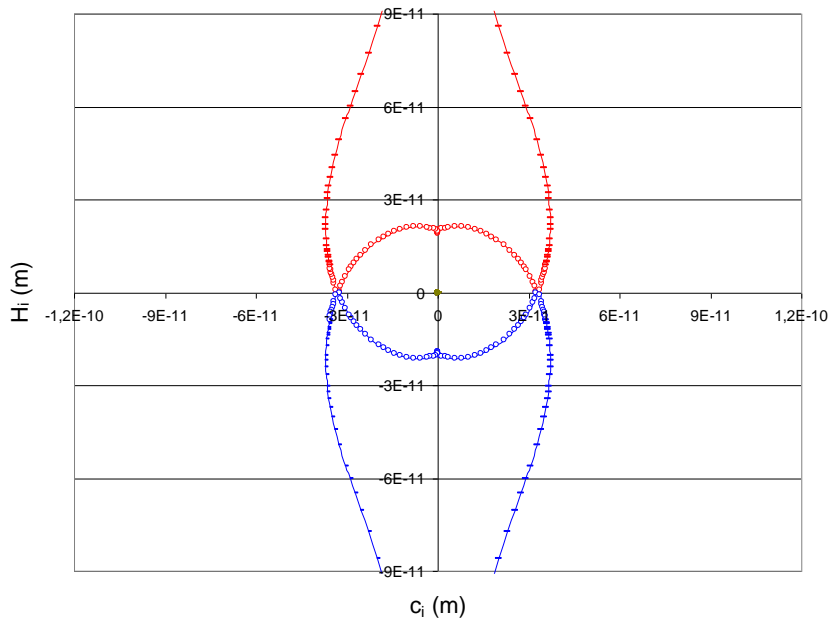
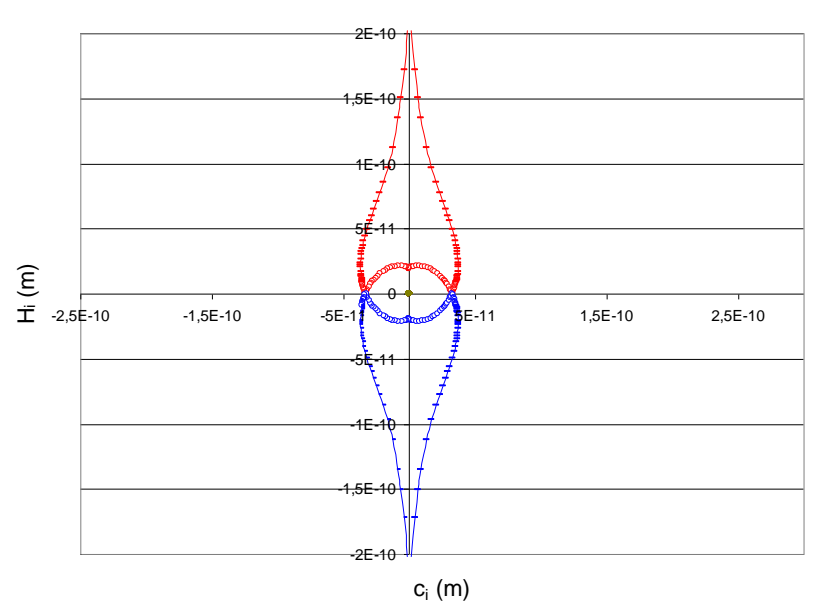


Figure 6 -  $2p^3$  Nitrogen with  $C_{POTI-AL}$





## P28 Free passage in OPA (OPA jump) when $d \rightarrow \infty$ with geometric sign change.

### p lobe

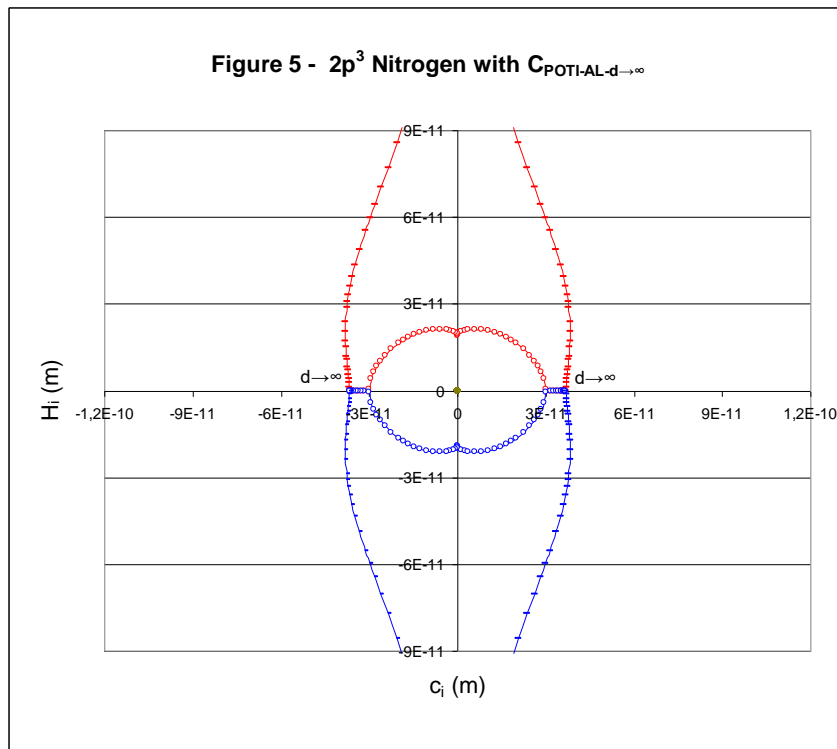
Electronic extremes cycle from  $d \rightarrow \infty$ , to  $d \rightarrow 1$  and back to  $d \rightarrow \infty$ . After this cycle,  $H_i$  sign is modified and, if first cycle is with  $H_i$  positive sign, second cycle is with  $H_i$  negative sign allowing existence of lobe painted in blue. Cycles alternate their  $H_i$  signs and run in  $C_{POTI}$  continuous modification from  $C_{POTI} \rightarrow 0$  to  $C_{POTI-GAL}$  or  $C_{POTI}$  geometric angular limit P033 [5]. When lobe is p-type,  $H_i$  sign modification is geometric sign change indicated in P28.

In this article end and by way of example, lobes are represented with three possible  $C_{POTI-GAL}$ :

- $C_{POTI-AL}$  (P032  $C_{POTI-AL}$  angular limit [5]) (Figures 5 and 6)
- $C_{POTI-LAG}$  (P031  $C_{POTI}$  lobe always growing [5]) in **Figures 7 and 8.**
- $C_{POTI-AL-d \rightarrow \infty}$  [5]. Option to pass "by contact" with  $C_{POTI-AL-d \rightarrow \infty}$  is represented in **Figure 5.B.** In  $C_{POTI-AL-d \rightarrow \infty}$  is "by contact" because both electronic extremes, A and B, are found in contact (in the same position) and from this position other cycle is initiated.

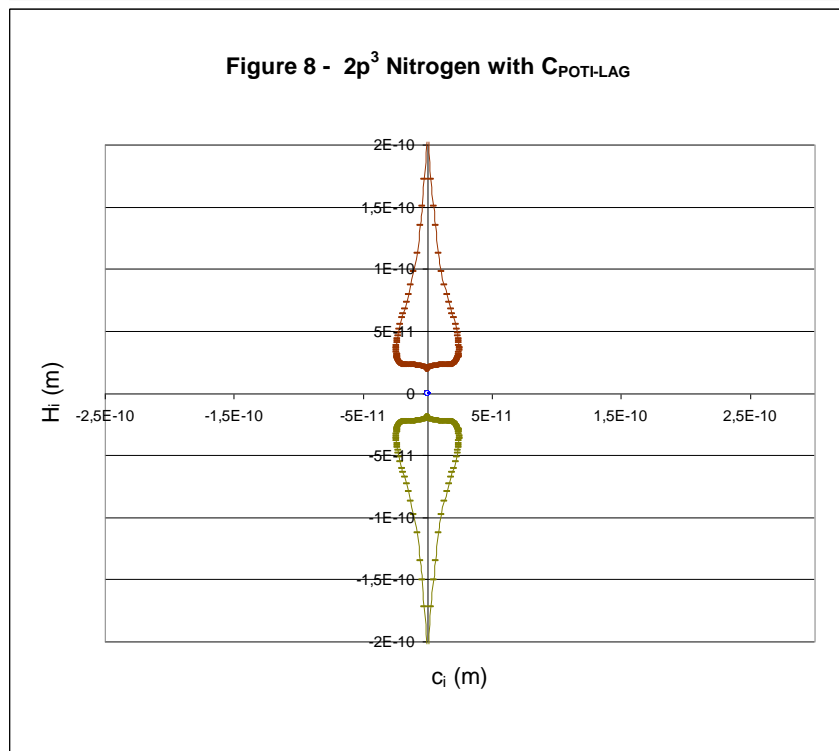
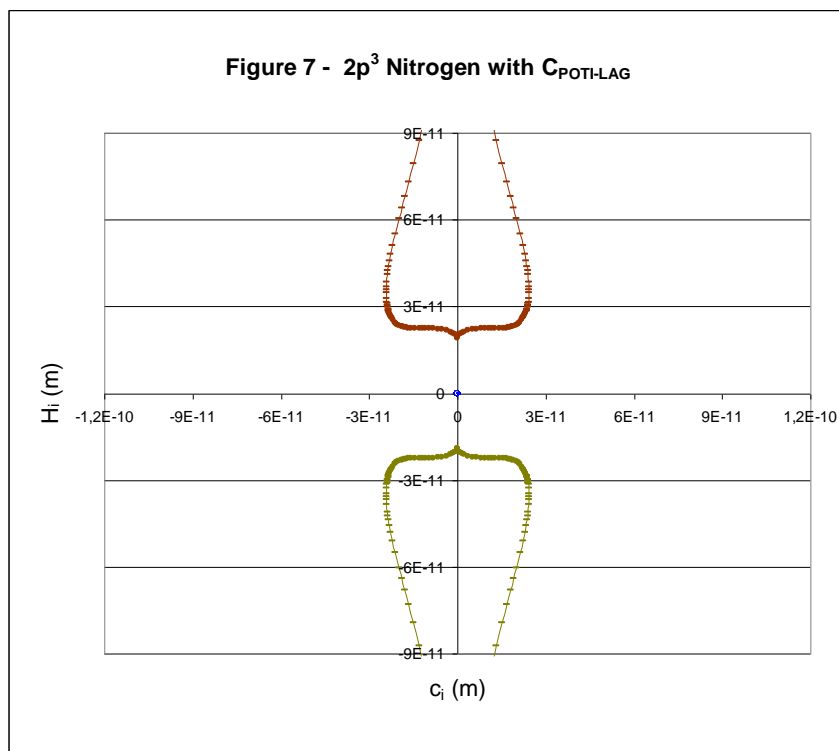
Advantage is that both electronic extremes are in same position and is position for change cycle.

Disadvantage is that B divisions that have no real value should be justified.



In five figures, A and B electronic extremes with same  $H_i$  sign are in identical colour. B intern electronic extreme divisions are with empty circles and A extern electronic extreme divisions are with horizontal to be differentiated. Symbol change point is  $d \rightarrow \infty$ .

Note: P28 is postulated number jumped between [3] and [4]



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## 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. 8 is present article. Jump from "Article 09" to "Article 20" is consequence of second part inclusion.

Abbreviations Table						
Abbreviation	6	7	8	9	20	Meaning
$\alpha_{NOA}$		X				Nucleus-Orbit-Angle
$a_0$						Bohr radius
AL						Angular Limit
BES	X	X	X	X		Born Electronic System
$c_i$	X	X	X	X		EE Orbital circumference
$C_F$	X		X	X		Wavelength compaction factor
$C_{MON}$	X	X				$C_F$ without $C_{POTI}$
$C_{PEP}$	X	X	X	X		Probability electrons pair coefficient
$C_{POTI}$	X	X	X	X		Probabilistic Orbital Tide in Third Feliz Solution
$C_{POTI-AL}$		X	X	X		$C_{POTI}$ Angular Limit
$C_{POTI-GAL}$			X			$C_{POTI}$ Geometric Angular Limit
$C_{POTI-LAG}$			X			$C_{POTI}$ Lobe always growing

d	X	X	X	X	Birth wavelength division or simply, division
EE	X	X	X	X	Electronic extreme
E <sub>o</sub>	X	X	X	X	Initial, birth or output energy
E <sub>i</sub>			X		EE energy
f	X				Constant in Victoria Equation
F		X			Constant f multiplied by z
GAL					Geometric Angular Limit
GNC	X	X	X	X	Geometric NIN Coupling
ħ	X		X		Reduced Planck's constant
h <sub>i</sub>					Planck's constant adapted to EE
H <sub>i</sub>	X	X	X	X	EE Circular orbit height
IE	X	X	X	X	Ionization Energy
m <sub>e</sub>			X		Electron mass
m <sub>i</sub>					EE mass
J	X				C <sub>F</sub> order in Second Feliz Solution (From x=1 to J)
K <sub>P</sub>					Probability constant in Variable C <sub>F</sub>
λ <sub>Birth</sub> λ		X	X		Birth wavelength
M	X				MON (Modified Orbital Number)
MON	X	X	X	X	Modified Orbital Number
NIN	X	X	X	X	Negative in Negative (Electron in electron concept)
OES	X	X	X	X	Origin Electronic System
OPA			X		Orbital Planes Axis
P <sub>i</sub>	X	X	X	X	EE Probability
P	X				PEP (Principal Electronic Part)
PEP	X				Principal Electronic Part
PNC	X	X	X	X	Probabilistic NIN Coupling
P <sub>Y to X</sub>	X				P <sub>y</sub> with respect to X lobe
r <sub>i</sub>	X	X	X	X	Distance between nucleus and EE
v <sub>i</sub>			X		EE velocity
z	X	X	X	X	Effective nuclear charge
Z		X	X		Atomic number

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