cubic ellipsoid nucleus - atomic physics - part 3: electronegativity

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Abstract

This work describes electronegativity in the light of the cubic ellipsoid nuclear model.
Its main statement is that the electronegativity depends on the number of protons in the uppermost unclosed nuclear shell and the shielding.
According to the ellipsoid nuclear model [10], the nuclear shells correlate with the atomic shells (unlike the common nuclear shell model); based on this assumption and the former articles regarding the atomic radius [11] and the ionization energy [12], we get to the following conclusions:

- The protons have no effect on the electrons beyond their correlated atomic shell.
- Moreover possibly the protons only affect the electrons that correlate with their shell.
- A physical theoretical electronegativity function was constructed to meet these requirements.
- The nuclear structure determines the atomic shape and the electronic shielding; this explains the variation of the electronegativity from the calculated value and links between the nuclear and atomic structure.

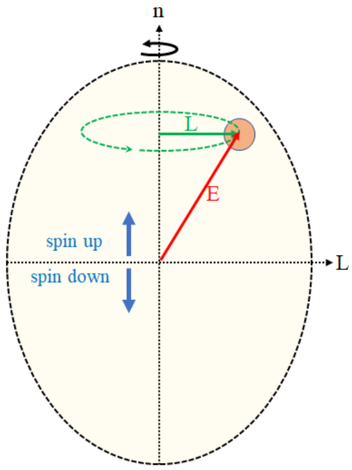
Content

The model at a glance

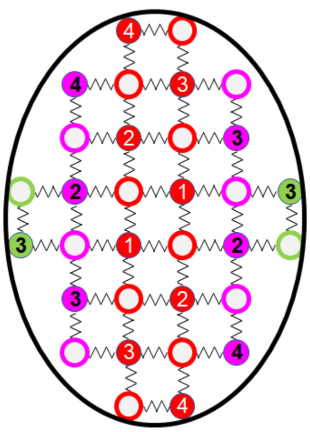
According to the model these are the shape and properties of the nucleus:

- the nucleus has an ellipsoid shape.
- the nucleon bonds build a cubic system.
- protons are connected to neutrons (**p-n**).
- neutrons are connected mainly to protons.
- the protons are populated and organized in shells in the nucleus in analogy to those of the electrons in the atom.
- the energy layers (principal quantum number **n**) grow with the distance from the origin.
- the perpendicular distance from the **z**-axis in the **x-y**-plane reflects the angular momentum (**L**, sub-orbitals).
- the upper half of the ellipsoid is referred to as spin-up and the lower part as spin-down.
- the nucleus possibly rotates around its **z**-axis.

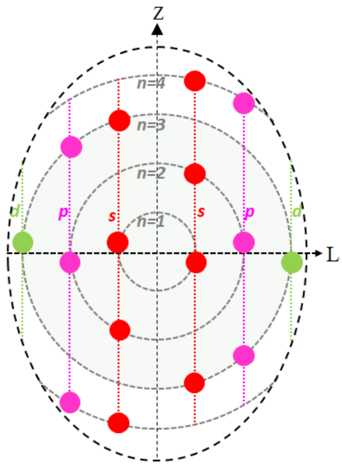
The following drawings describe the idea via cross sections in the **x-z**-plane of the nucleus.



***1**: a nucleon in the nucleus*



***2**: the bonds between the nucleons*

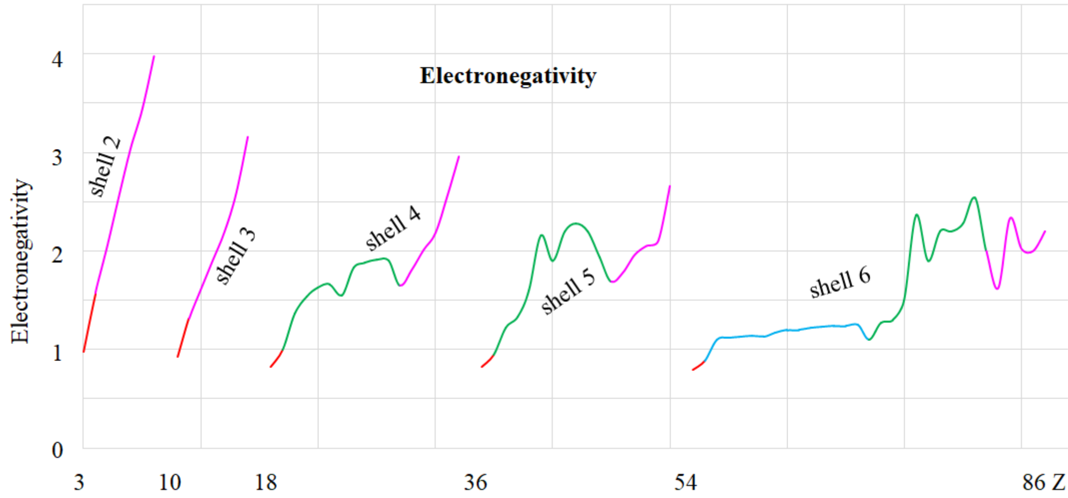


***3**: the energy levels of the nucleus*

1. a nucleon (**circle**) is observed inside the ellipsoid (dashed line) that encloses the nucleons and schematically defines the nuclear surface:
   - the distance from the origin represents its energy **E**.
   - the distance from the **z**-axis depicts it angular momentum **L**.
   - the nucleons in the upper half have spin-up, and in the lower one spin-down.
2. the bonds between the nucleons are shown for visibility as springs.
   - **protons**: full circles of the **s**, **p** and **d** sub-orbitals. **neutrons**: hollow circles.
3. the circles of equal energy states **n** in the ellipsoid.
   - the lines mark the development of the **s**, **p** and **d** sub-orbitals along the **z**-axis.
   - the **s** line crosses all **n** circles from 1 to 4 (**s1** to **s4**).
   - the **p** line begins by **n**=2 and reaches till **n**=4 (**p2** to **p4**).
   - the **d** line begins by **n**=3 and reaches the ellipsoid border, before it reaches the **n**=4 circle, and therefore there are no **d4** states at this stage (only **d3**).

Introduction

In the former studies of the atomic radius [10] and ionization energy [11], we raised the assumption, that each nuclear layer influences only its relevant electronic layer and so the attraction outside the atom can only be due to an unclosed outermost layer [10], [11]. This attraction force is proportional to the number of protons in the outermost layer.
The following graph shows the data of the electronegativity of the elements as a function of the atomic number [2]:



The area through which the force is getting out of the atom, is the one where protons are missing.
We therefore assume the following:

- Electronegativity is related to the number of protons in the outermost, non-closed nuclear shell.
- The fewer layers the atom has, the less shielding it has and the greater its electronegativity.

The research

Constructing the electronegativity function

Electronegativity is a measure for the attraction of electrons by an atom in a chemical bond; it depends on:

- the number of protons in the outermost, non-closed nuclear shell.
- the shielding.

It is reminded here again that according to the model, the nuclear and atomic shells correspond to each other, and are as they appear in the periodic system.
We follow similar steps to those we took in the former studies of the atomic radius [10] and ionization energy [11].
We define:

- χ_0: offset of the electronegativity.
- Z: the atomic number of the atom observed.
- $k \in \{1, 2, 3, 4, 5, 6, 7\}$ the current nuclear (and atomic) shell.
- Z_{shell_k}: the number of protons (or electrons) currently in the shell, meaning:
- $Z_{shell_k} = Z - Z_{n.g_{k-1}}$.
- $Z_{n.g_{k-1}}$: the (noble gas) atomic number that closes the last row of the periodic table.
- a: slope.
- b: shielding coefficient.
- $\exp(n, L)$: shielding exponent (depends on the shell n and the sub-orbital l).

and estimate the electronegativity as a function of the number of protons in the outermost nuclear shell:

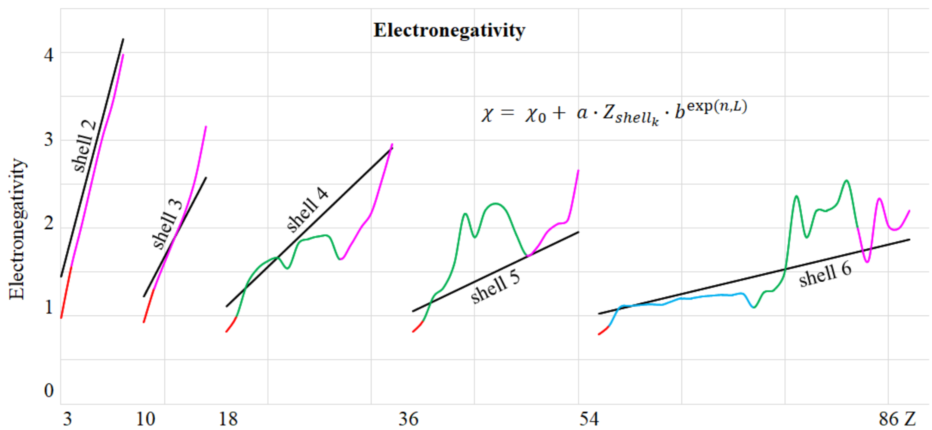
- χ grows with Z_{shell_k}: $\chi \sim Z_{shell_k}$
- the shielding depends on the atomic shell and sub-orbital.

We therefore try the simplified function: $\chi = \chi_0 + a \cdot Z_{shell_k} \cdot b^{\exp(n,L)}$
and obtain by tests the values:

- $\chi_0 \approx 1.0$
- $a \approx 0.9$
- $b \approx 0.5$
- $\exp(n, L) \approx \{0, 1, 2, 3, 3, 4\}$

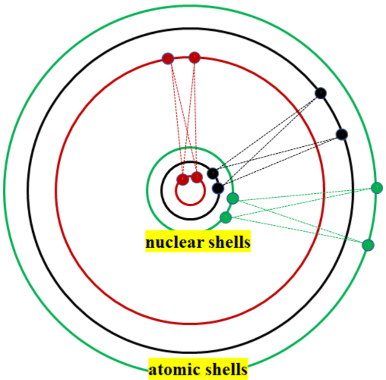
Analysis of the electronegativity

The electronegativity function agrees well with the data. The variation seems to be mainly due to shielding effects and the sub-orbitals, that are not taken directly into account in the function.
The shielding is discussed in detail in the appendix.



***graph**: data of the electronegativity (**S**, **P**, **D**, **F** sub-orbitals); dotted line: calculated function*

According to the electronegativity function, protons appear to have no effect on electrons beyond their correlated atomic shell; it seems that also below their shells they have no influence.
We get to the conclusion, that according to this simplified model at least, each atomic shell is influenced only by its correlated nuclear shell.
The following illustration depicts this idea.



each nuclear shell affects only its corresponding atomic shell

This conclusion agrees with our former research, regarding the atomic radius and the ionization energy [11], [12].

Discussion of the results and conclusions

Based on our studies of the atomic radius [11] and the ionization energy [12] and the assumption that the nuclear and atomic shells fully correlate, as our initial research suggests [10], we conclude that the electronegativity depends mainly on the number of protons in the outermost nuclear shell and the atomic shielding.
Next study uses this result to understand the bond angles of the atom in chemical compounds.

Sources and references

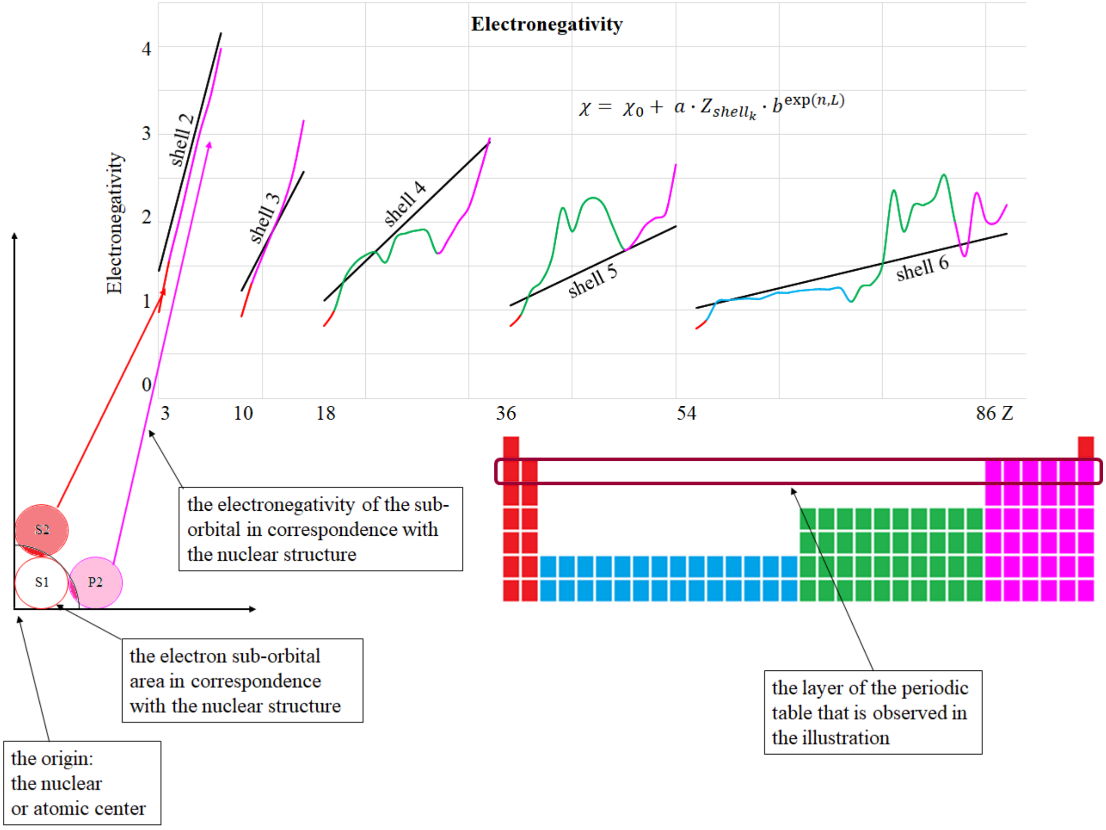
1. *Electronegativity - Wikipedia*
2. *List of Electronegativity Values of the Elements - Science Notes*
3. *Binding energy - Wikipedia*
4. *Intramolecular force - Wikipedia*
5. *Ionic bonding - Wikipedia*
6. *Covalent bond - Wikipedia*
7. *Metallic bonding - Wikipedia*
8. *Intermolecular force - Wikipedia*
9. *Van Arkel-Ketelaar triangle - Wikipedia*
10. *cubic ellipsoid nucleus - part 1 - the model and its mass formula - Ronen Yavor*
11. *cubic ellipsoid nucleus - atomic physics - part 1 - the atomic radius - Ronen Yavor*
12. *cubic ellipsoid nucleus - atomic physics - part 2 - the ionization energy - Ronen Yavor*

Appendix

graphs

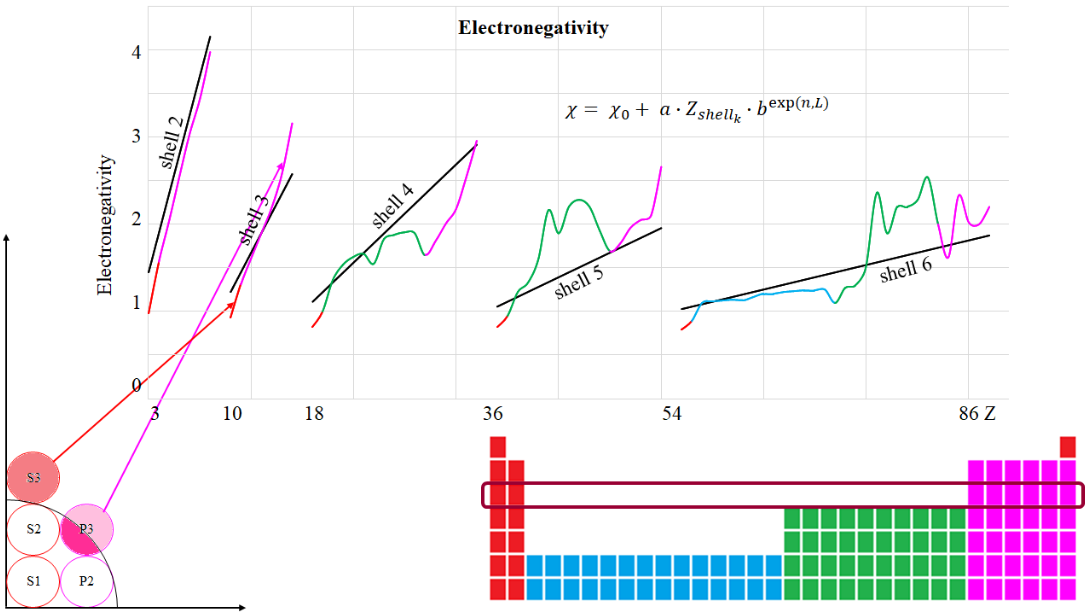
Following graphs discuss the electronegativity.

Electronegativity - row 2
The **S**-2 and P-2 orbitals are shielded almost equally by the **S**-1.
The electronegativity grows linearly with the number of protons in the nucleus.



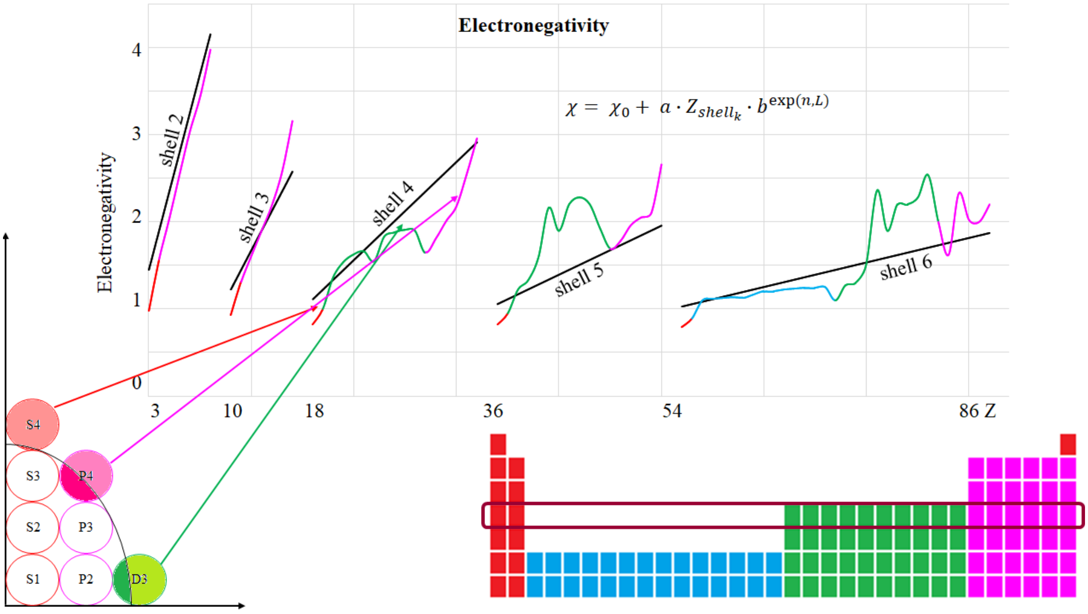
Electronegativity - row 3

The P-3 orbital is less shielded than the **S**-3 orbital, the difference is small, so basically the electronegativity grows with the number of protons, yet a bit stronger for the P-3 orbital.



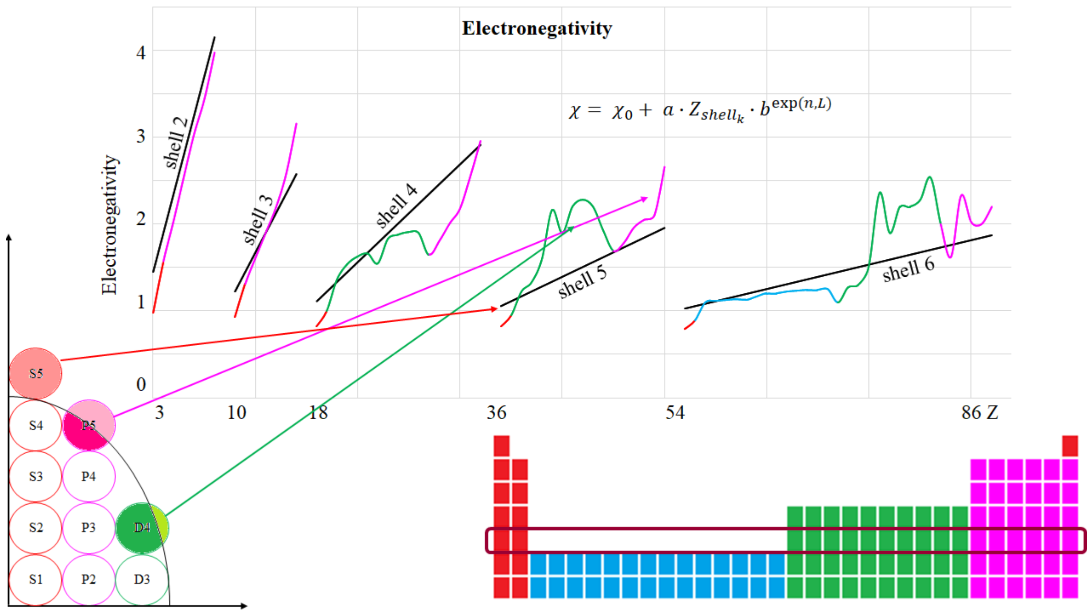
Electronegativity - row 4

The **D**-3 is less shielded and therefore its electronegativity is a bit above the curve.



Electronegativity - row 5

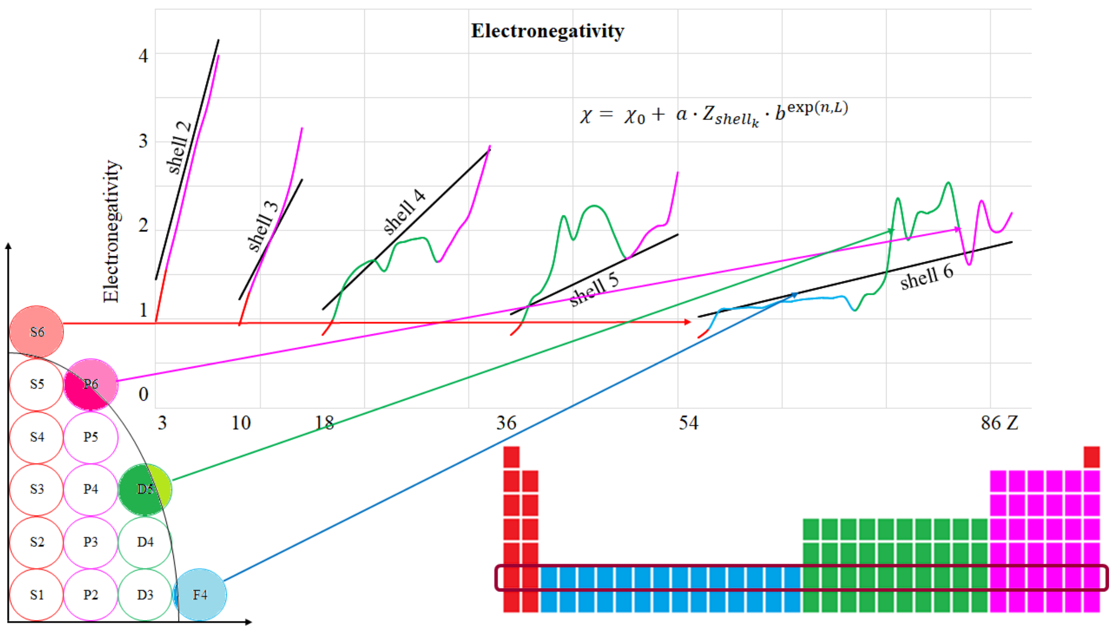
The D-4 is less shielded and therefore its electronegativity is a bit above the curve.



Electronegativity - row 6

The F-4 orbital is shielded and so lies somewhat below the curve.

The D-5 and P-6 lie above, because they are less shielded.



data

the electronegativity function was defined as:

- χ_0: offset of the electronegativity.
- Z: the atomic number of the atom observed.
- $k \in \{1, 2, 3, 4, 5, 6, 7\}$ the current nuclear (and atomic) shell.
- Z_{shell_k}: the number of protons (or electrons) currently in the shell, meaning:
- $Z_{shell_k} = Z - Z_{n.g_{k-1}}$.
- $Z_{n.g_{k-1}}$: the (noble gas) atomic number that closes the last row of the periodic table.
- a: slope.
- b: shielding coefficient.
- $\exp(n, L)$: shielding exponent (depends on the shell n and the sub-orbital l).

and estimate the electronegativity as a function of the number of protons in the outermost nuclear shell:

- χ grows with Z_{shell_k}: $\chi \sim Z_{shell_k}$
- the shielding depends on the atomic shell and sub-orbital.

We therefore try the simplified function: $\chi = \chi_0 + a \cdot Z_{shell_k} \cdot b^{\exp(n,L)}$
and obtain by tests the values:

- $\chi_0 \approx 1.0$
- $a \approx 0.9$
- $b \approx 0.5$
- $\exp(n, L) \approx \{0, 1, 2, 3, 3, 4\}$

Data Table
The following table contains the data.
Legend:

- exp_{shell}: the shielding exponent (of b)

symbol	Z	Z_{shell}	Z_{row}	sub orbital	exp_{shell}	calc	data
H	1	0	1	s	0		
He	2	2	2	s	0		
Li	3	2	1	s	1	1.45	0.98
Be	4	2	2	s	1	1.90	1.57
B	5	2	3	p	1	2.35	2.04
C	6	2	4	p	1	2.80	2.55
N	7	2	5	p	1	3.25	3.04
O	8	2	6	p	1	3.70	3.44
F	9	2	7	p	1	4.15	3.98
Ne	10	10	8	p	1		
Na	11	10	1	s	2	1.23	0.93
Mg	12	10	2	s	2	1.45	1.31
Al	13	10	3	p	2	1.68	1.61
Si	14	10	4	p	2	1.90	1.90
P	15	10	5	p	2	2.13	2.19
S	16	10	6	p	2	2.35	2.58
Cl	17	10	7	p	2	2.58	3.16
Ar	18	18	8	p	2		
K	19	18	1	s	3	1.11	0.82
Ca	20	18	2	s	3	1.23	1.00
Sc	21	18	3	d	3	1.34	1.36
Ti	22	18	4	d	3	1.45	1.54
V	23	18	5	d	3	1.56	1.63
Cr	24	18	6	d	3	1.68	1.66
Mn	25	18	7	d	3	1.79	1.55
Fe	26	18	8	d	3	1.90	1.83
Co	27	18	9	d	3	2.01	1.88
Ni	28	18	10	d	3	2.13	1.91
Cu	29	18	11	d	3	2.24	1.90
Zn	30	18	12	d	3	2.35	1.65
Ga	31	18	13	p	3	2.46	1.81
Ge	32	18	14	p	3	2.58	2.01
As	33	18	15	p	3	2.69	2.18
Se	34	18	16	p	3	2.80	2.55
Br	35	18	17	p	3	2.91	2.96
Kr	36	36	18	p	3		
Rb	37	36	1	s	4	1.06	0.82
Sr	38	36	2	s	4	1.11	0.95
Y	39	36	3	d	4	1.17	1.22
Zr	40	36	4	d	4	1.23	1.33
Nb	41	36	5	d	4	1.28	1.60
Mo	42	36	6	d	4	1.34	2.16
Tc	43	36	7	d	4	1.39	1.90
Ru	44	36	8	d	4	1.45	2.20
Rh	45	36	9	d	4	1.51	2.28
Pd	46	36	10	d	4	1.56	2.20
Ag	47	36	11	d	4	1.62	1.93
Cd	48	36	12	d	4	1.68	1.69
In	49	36	13	p	4	1.73	1.78
Sn	50	36	14	p	4	1.79	1.96
Sb	51	36	15	p	4	1.84	2.05

symbol	Z	Z_{shell}	Z_{row}	sub orbital	exp_{shell}	calc	data
Te	52	36	16	p	4	1.90	2.10
I	53	36	17	p	4	1.96	2.66
Xe	54	54	18	p	4		
Cs	55	54	1	s	5	1.03	0.79
Ba	56	54	2	s	5	1.06	0.89
La	57	54	3	f	5	1.08	1.10
Ce	58	54	4	f	5	1.11	1.12
Pr	59	54	5	f	5	1.14	1.13
Nd	60	54	6	f	5	1.17	1.14
Pm	61	54	7	f	5	1.20	1.13
Sm	62	54	8	f	5	1.23	1.17
Eu	63	54	9	f	5	1.25	1.20
Gd	64	54	10	f	5	1.28	1.20
Tb	65	54	11	f	5	1.31	1.22
Dy	66	54	12	f	5	1.34	1.23
Ho	67	54	13	f	5	1.37	1.24
Er	68	54	14	f	5	1.39	1.24
Tm	69	54	15	f	5	1.42	1.25
Yb	70	54	16	f	5	1.45	1.10
Lu	71	54	17	d	5	1.48	1.27
Hf	72	54	18	d	5	1.51	1.30
Ta	73	54	19	d	5	1.53	1.50
W	74	54	20	d	5	1.56	2.36
Re	75	54	21	d	5	1.59	1.90
Os	76	54	22	d	5	1.62	2.20
Ir	77	54	23	d	5	1.65	2.20
Pt	78	54	24	d	5	1.68	2.28
Au	79	54	25	d	5	1.70	2.54
Hg	80	54	26	d	5	1.73	2.00
Tl	81	54	27	p	5	1.76	1.62
Pb	82	54	28	p	5	1.79	2.33
Bi	83	54	29	p	5	1.82	2.02
Po	84	54	30	p	5	1.84	2.00
At	85	54	31	p	5	1.87	2.20
Rn	86	86	32	p	5		