New quantization method to calculate the energy levels of the atoms: the modified potencial Coulomb energy – Part 1

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Abstract

To explain the energy levels of the atoms, we use a new equation of quantization. This equation is a modified potencial Coulomb energy multiplied by the period which has the SI unit of angular moment (J.s). The calculations are in agreement for the atoms of H, He, Li, Be and C. The maximum error is 3.6% but only using the Coulomb force. It is necessary to continue the research for the others forces too.

1. Introduction

The calculation of the energy levels of H, He, Li, Be and C are in the next sections. They are in agreement with the experimental energy between an error of 3.6%, see table 1 and 2. In the calculations we compute only the Coulomb force.

Atom	Z	e^-	E (eV) theoret.	E (eV) exper.	Error %
H I	1	1	13.6	13.6	0.0
He I	2	2	78.7	79.0	-0.4
He II	2	1	54.4	54.4	0.0
Li I	3	3	196.0	203.4	-3.6
Li II	3	2	200.1	198.0	1.5
Li III	3	1	122.4	122.4	0.0
Be I	4	4	385.2	399.1	-3.5
Be II	4	3	386.8	389.8	-0.8
Be III	4	2	377.6	371.6	1.6
Be IV	4	1	217.6	217.7	0.0
C I	6	6	998.4	1030.1	-3.1
C III	6	4	992.2	994.5	-0.2
C IV	6	3	951.3	946.6	0.5
C V	6	2	894.5	882.1	1.4
C VI	6	1	489.8	490.0	0.0

Table 1 . Atom energies theoretical and experimental of H, He, Li, Be and C. Experimental values from [1].

		Error (%) $\left(\frac{E_{theoret.}}{E_{\exp erim.}}-1\right)100$				
	Z	Atom with 1 e-	Atom with 2 e-	Atom with 3 e-	Atom with 4 e-	Atom with 6 e-
H	1	0.0				
He	2	0.0	-0.4			
Li	3	0.0	1.5	-3.6		
Be	4	0.0	1.6	-0.8	-3.5	
B	5	0.0	1.5	0.1	-1.2	
C	6	0.0	1.4	0.5	-0.2	-3.1
N	7	0.0	1.3	0.7	0.3	-1.1
O	8	0.0	1.2	0.7	0.5	-0.1
F	9	0.0	1.1	0.7	0.7	0.5
Ne	10	0.0	1.0	0.7	0.7	0.9
Ca	20	0.0	0.6	0.5	0.7	1.3
Zn	30	0.0	0.4	0.4	0.6	1.1
ZR	40	0.0	0.4	0.4	0.5	1.0
Sn	50	0.1	0.4	0.4	0.5	0.9
Hg	80	0.3	0.5	0.5	0.5	0.8
Fm	100	0.6	0.9	0.6	0.5	0.5

Table 2 . Error in % between the atom energies theoretical and experimental. The atoms are for 1 electron (for exemple: Fm C), 2 electrons (Fm XCIX), 3 electrons (Fm XCVIII), 4 electrons (Fm XCVII) and 6 electrons (Fm XCV).

The atoms of the Table 1 are the simplest of calculating because the eletrons are symmetrical.

In the development we used the Newtonian equations. In Section 7 we have the relativistic correction. All the tables are with the relativistic correction.

The method of calculation is described below. We use the HeI as example.

1.1. The equation of forces for the HeI and for a circular path of the electrons is:

$$m\frac{v^2}{r}=\frac{e^2}{4\pi\varepsilon_o}\left(\frac{2}{r^2}-\frac{1}{(2r)^2}\right) \qquad (1)$$

1.2. The new equation of quantization is:

$$V_{qu.}T=nh \qquad [\text{J.s}] \qquad (2)$$

where T is the period and $V_{qu.}$ is the equation of Coulomb force with the denominator of the right term without being high to the square and in scalar form. For the He I is:

$$V_{qu.} = \frac{e^2}{4\pi\varepsilon_o}\left(\frac{2}{r} - \frac{1}{2r}\right) \quad (3)$$

1.3. The modified equation of energy for each electron is:

$$V_{m.e1} = V_{m.e2} = -\frac{Ze^2}{4\pi\varepsilon_o} = -\frac{e^2}{4\pi\varepsilon_o}\frac{2}{r} \quad (4)$$

so, the modified potencial energy is the atom nucleus charge (Ze^2) divided by the radius r and the Coulomb constant..

1.4. The energy calculated for the HeI is

$$E = K_{e1} + K_{e2} + V_{m.e1} + V_{m.e2} \quad (5)$$

where K_e is the kinetic energy. For low velocities we have:

$$K_e = \frac{1}{2}mv^2 \quad (6)$$

where $V_{qu.}T$ has the SI unit of angular momentum [J.s], n is the quantization number, h is the Planck constant, r is the distance between the nucleus and the electron, Ze is the charge, $1/4\pi\varepsilon_o$ is the Coulomb constant and m and v are respectively the mass and the velocity of the electron.

2. Hydrogen atom

For the hydrogen neutral atom (1 protons and 1 electron), for circular path of the electron the forces are:

$$m\frac{v^2}{r} = \frac{e^2}{4\pi\varepsilon_o}\frac{1}{r^2}$$

$$mv^2 r = \frac{e^2}{4\pi\varepsilon_o} \quad (7)$$

The period is:

$$T = \frac{2\pi r}{v} = \xi\Delta t \quad (8)$$

where ξ is an experimental data and for hydrogen atom is $\xi/2\pi = 1/\alpha \cong 1/137$, α is the fine structure constant and

$$\Delta t = \frac{r}{c} \qquad (9)$$

where c is the velocity of light.
Substituting (8) in (7) we have:

$$mv^3 \frac{T}{2\pi} = \frac{e^2}{4\pi\varepsilon_o} \qquad (10)$$

Substituting (8) in (10) we have:

$$mv^3 \xi \Delta t = \frac{2\pi e^2}{4\pi\varepsilon_o} \qquad (11)$$

Substituting (9) in (11) we have:

$$mv^3 \xi r = c2\pi \frac{e^2}{4\pi\varepsilon_o} \qquad (12)$$

Dividing (12) and (7) we have:

$$\xi = \frac{2\pi c}{v} \qquad (13)$$

Substituting (13) in (7) we have:

$$r = \frac{e^2}{4\pi\varepsilon_o} \frac{1}{m} \left(\frac{\xi}{2\pi c} \right)^2 \qquad (14)$$

From Section 1.2 we have:

$$V_{qu.} = \frac{e^2}{4\pi\varepsilon_o} \frac{1}{r} \qquad (15)$$

which for H is the potencial Coulomb energy.
Multiplying (15) and (8) we have:

$$V_{qu.} T = \frac{e^2}{4\pi\varepsilon_o} \frac{1}{r} \xi \Delta t \qquad (16)$$

Substituting (9) in (16) we have :

$$V_{qu.}T = \frac{1}{4\pi\varepsilon_o}\frac{e^2}{c}\xi = nh \qquad \text{[J.s]} \qquad (17)$$

Substituting (17) in (14) we have:

$$r = \frac{4\pi\varepsilon_o}{e^2}\frac{n^2\hbar^2}{m} \qquad (18)$$

Substituting (18) in (7) we have:

$$v = \frac{e^2}{4\pi\varepsilon_o}\frac{1}{n\hbar} \qquad (19)$$

From Section 1.3 we have:

$$V_{m.e} = -\frac{1}{4\pi\varepsilon_o}\frac{e^2}{r}$$

which for H is the potencial Coulomb energy. The total energy of H is:

$$E = K_e + V_{m.e} = \frac{1}{2}mv^2 - \frac{e^2}{4\pi\varepsilon_o}\frac{1}{r} \qquad (20)$$

Substituting (18) and (19) in (20) we have:

$$E = -K_e = -\frac{me^4}{(4\pi\varepsilon_o)^2 2\hbar^2}\frac{1}{n^2} \qquad (21)$$

The total energy for H is:

$$E = -\frac{1}{2}27.2 = -13.6 \text{ eV}$$

Equations (18), (19) and (21) are the same of Bohr and are in agreement with the experiments for the hydrogen atom.

3. Helium atom

3.1 – He I

For the He I atom (2 protons and 2 electrons) and for circular path of the electron the forces are:

$$m\frac{v^2}{r} = \frac{e^2}{4\pi\varepsilon_o}\left(\frac{2}{r^2} - \frac{1}{(2r)^2}\right)$$

$$mv^2 r = \frac{7}{4}\frac{e^2}{4\pi\varepsilon_o} \qquad (22)$$

Making the same sequence of calculation from (8) to (12) we have the same equation for the He I:

$$\xi = \frac{2\pi c}{v} \qquad (23)$$

Substituting (23) in (22) we have:

$$r = \frac{7}{4}\frac{e^2}{4\pi\varepsilon_o}\frac{1}{m}\left(\frac{\xi}{2\pi c}\right)^2 \qquad (24)$$

From Section 1.2 we have:

$$V_{qu.} = \frac{e^2}{4\pi\varepsilon_o}\left(\frac{2}{r} - \frac{1}{2r}\right) = \frac{3}{2}\frac{e^2}{4\pi\varepsilon_o}\frac{1}{r} \qquad (25)$$

Multiplying (25) and (8) we have:

$$V_{qu.}T = \frac{3}{2}\frac{e^2}{4\pi\varepsilon_o}\frac{\xi\Delta t}{r} \qquad (26)$$

Substituting (9) in (26) we have:

$$V_{qu.}T = \frac{3}{2}\frac{e^2}{4\pi\varepsilon_o}\frac{\xi}{c} = nh \qquad (27)$$

Substituting (27) in (24) we have:

$$r = \frac{7}{9}\frac{4\pi\varepsilon_o}{e^2}\frac{n^2\hbar^2}{m} \qquad (28)$$

Substituting (28) in (22) the velocity of electron 1 (e_1) and electron 2 (e_2) is:

$$v^2 = \frac{9}{4}\frac{e^4}{(4\pi\varepsilon_o)^2}\frac{1}{n^2\hbar^2} \qquad (29)$$

$$K_{e1} = 0.5\frac{9}{4}\frac{e^4}{(4\pi\varepsilon_o)^2}\frac{m}{n^2\hbar^2}$$

From section 1.3 we have:

$$V_{m.e1} = V_{m.e2} = -\frac{Ze^2}{4\pi\varepsilon_o r} = -\frac{e^2}{4\pi\varepsilon_o}\frac{2}{r} \qquad (30)$$

Substituting (28) in (30) we have:

$$V_{m.e1} = V_{m.e2} = -\frac{18}{7}\frac{e^4}{(4\pi\varepsilon_o)^2}\frac{m}{n^2\hbar^2} \qquad (31)$$

The total energy of the HeI is:

$$E = K_{e1} + K_{e2} + V_{m.e1} + V_{m.e2}$$

$$E = 2\left(\frac{9}{8} - \frac{18}{7}\right)x27.2eV = -78.7 \text{ eV}$$

3.2 – He II

For the He II atom (2 protons and 1 electron), for circular path of the electron the forces are:

$$mv^2 r = 2\frac{e^2}{4\pi\varepsilon_o}$$

From section 1.2 for e1 is:

$$V_{qu.} = \frac{e^2}{4\pi\varepsilon_o}\frac{2}{r}$$

From section 1.3 we have:

$$V_{m.e1} = -\frac{e^2}{4\pi\varepsilon_o}\frac{2}{r}$$

Making the same sequence of calculation of the electron 1 from He we have:

$$r = \frac{1}{2}\frac{4\pi\varepsilon_o}{e^2}\frac{n^2\hbar^2}{m}$$

$$K_{e1} == \frac{1}{2}4\frac{e^4}{(4\pi\varepsilon_o)^2}\frac{1}{n^2\hbar^2}$$

$$V_{m.e1} = -4\frac{e^4}{(4\pi\varepsilon_o)^2}\frac{m}{n^2\hbar^2}$$

The total energy of the He II is:

$$E = K_{e1} + V_{m.e1}$$

$$E = (2-4)27.2eV = -54.4 \text{ eV}$$

4. Lithium atom

The lithium neutral atom has 3 protons and 3 electrons (Li I), see Figure 1.

4.1 – Electrons 1 and 2

The resulting force on electron 1 (see Figure 2) is::

$$F_{res.} = \frac{e^2}{4\pi\varepsilon_o}\frac{2.7362}{r^2}$$

The angle $\theta = 1.095°$ is small and we will consider a central force and a circular path. So, the forces for electron 1 and 2 are:

$$m\frac{v^2}{r} = \frac{e^2}{4\pi\varepsilon_o}\frac{2.7362}{r^2}$$

$$mv^2 r = 2.7362\frac{e^2}{4\pi\varepsilon_o}$$

From Section 1.2 for e_1 and e_2 is:

$$V_{qu.1.e} = \frac{e^2}{4\pi\varepsilon_o}\left(\frac{3}{r} - \frac{1}{2r} - \frac{1}{4.1231r}\right) = 2.2575\frac{e^2}{4\pi\varepsilon_o}\frac{1}{r}$$

From section 1.3 we have:

$$V_{m.e1} = V_{m.e2} = -\frac{Ze^2}{4\pi\varepsilon_o r} = -\frac{e^2}{4\pi\varepsilon_o}\frac{3}{r}$$

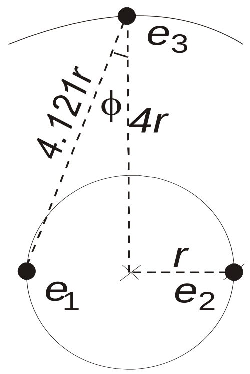

Figure1 – Lithium neutral atom with 3 electrons

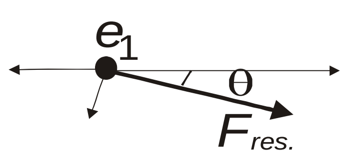

Figure 2 – The resulting force $F_{res.}$ on the electron 1

Making the same sequence of calculation of the electrons 1 and 2 of He we have:

$$r = 0.53689\frac{4\pi\varepsilon_o}{e^2}\frac{n^2\hbar^2}{m}$$

$$K_{e1} = K_{e2} = \frac{1}{2}5.0964\frac{e^4}{(4\pi\varepsilon_o)^2}\frac{m}{n^2\hbar^2}$$

$$V_{m.e1} = V_{m.e2} = -5.5877\frac{e^4}{(4\pi\varepsilon_o)^2}\frac{m}{n^2\hbar^2}$$

4.2 – Electron 3

The modified potencial energy for e3 is:

$$V_{m.e3} = \frac{V_{m.1e}}{n^2} = \frac{V_{m.1e}}{4} = -1.4003\frac{e^4}{(4\pi\varepsilon_o)^2}\frac{m}{\hbar^2}$$

The forces are:

$$m\frac{v^2}{4r} = \frac{e^2}{4\pi\varepsilon_o}\left(\frac{3}{(4r)^2} - \frac{2\cos 14.036}{(4.1231r^2)}\right)$$

$$mv^2 r = 0.29348\frac{e^2}{4\pi\varepsilon_o} \qquad (33)$$

Substituting (32) in (33) we have:

$$v^2 = 0.54794\frac{e^4}{(4\pi\varepsilon_o)^2}\frac{1}{n^2\hbar^2}$$

$$K_{e3} = K_{e2} = \frac{1}{2}0.54794\frac{e^4}{(4\pi\varepsilon_o)^2}\frac{m}{n^2\hbar^2}$$

The total energy of the Li I is:

$$E = K_{e1} + K_{e2} + K_{e3} + V_{m.e1} + V_{m.e2} + V_{m.e3}$$

$$E = [2x2.5482 + 0.27397 - 2x5.5877 - 1.4003]x27.2 = -196.0 \text{ eV}$$

5. Berilium atom

The berilium neutral atom has 4 protons and 4 electrons, see Fig. 3.

5.1 – Electrons 1 and 2

For circular trajectory we have the same equation of forces for electron 1 and 2:

$$m\frac{v^2}{r} = \frac{e^2}{4\pi\varepsilon_o}\left(\frac{4}{r^2} - \frac{1}{(2r)^2} - \frac{2sin14.036°}{(4.1231r)^2}\right)$$

$$mv^2 r = 3.7215\frac{e^2}{4\pi\varepsilon_o}$$

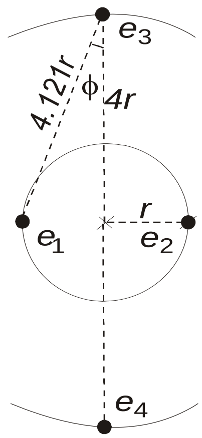

Figure 3 - Berilium neutral atom with 4 electrons

From Section 1.2 for e_1 and e_2 is:

$$V_{qu.1e} = \frac{e^2}{4\pi\varepsilon_o}\left(\frac{4}{r} - \frac{1}{2r} - \frac{1}{4.1231r}\right) = 3.015\frac{e^2}{4\pi\varepsilon_o}\frac{1}{r}$$

From section 1.3 we have:

$$V_{m.e1} = V_{m.e2} = -\frac{Ze^2}{4\pi\varepsilon_o r} = -\frac{e^2}{4\pi\varepsilon_o}\frac{4}{r}$$

Making the same sequence of calculation of the electrons 1 and 2 of He we have:

$$r = 0.4094\frac{4\pi\varepsilon_o}{e^2}\frac{n^2\hbar^2}{m} \qquad (34)$$

$$K_{e1} = K_{e2} = \frac{1}{2}9.0901\frac{e^4}{(4\pi\varepsilon_o)^2}\frac{m}{n^2\hbar^2}$$

$$V_{m.e1} = V_{m.e2} = -9.7704\frac{e^4}{(4\pi\varepsilon_o)^2}\frac{m}{n^2\hbar^2}$$

5.2 – Electron 3 and 4

The modified potencial energy for e3 and e4 is:

$$V_{m.e3} = V_{m.e4} = \frac{V_{m.1e}}{n^2} = \frac{V_{m.1e}}{4} = -2.4426 \frac{e^4}{(4\pi\varepsilon_o)^2} \frac{m}{\hbar^2}$$

The forces are:

$$m\frac{v^2}{4r} = \frac{e^2}{4\pi\varepsilon_o}\left(\frac{3}{(4r)^2} - \frac{1}{(8r)^2} - \frac{2\cos 14.036}{(4.1231r^2)}\right)$$

$$mv^2 r = 0.48098 \frac{e^2}{4\pi\varepsilon_o} \qquad (35)$$

Substituting (34) in (35) we have:

$$v^2 = 1.1748 \frac{e^4}{(4\pi\varepsilon_o)^2} \frac{1}{n^2\hbar^2}$$

$$K_{e3} = K_{e4} = \frac{1}{2} 1.1748 \frac{e^4}{(4\pi\varepsilon_o)^2} \frac{m}{n^2\hbar^2}$$

The total energy of the Li I is:

$$E = K_{e1} + K_{e2} + K_{e3} + K_{e4} + V_{m.e1} + V_{m.e2} + V_{m.e3} + V_{m.e4}$$

$$E = 2(4.545 + 0.5874) - 2(9.7704 + 2.4426)27.2 = -385.2 \text{ eV}$$

6. Carbon atom

The carbon neutral atom has 6 protons and 6 electrons, see Fig. 4.

6.1 – Electrons 1 and 2

For circular trajectory we have the same equation of forces for electron 1 and 2:

$$m\frac{v^2}{r} = \frac{e^2}{4\pi\varepsilon_o}\left(\frac{6}{r^2} - \frac{1}{(2r)^2} - \frac{1}{(5r)^2} + \frac{1}{(3r)^2} - \frac{2 sin 14.036°}{(4.1231r)^2}\right)$$

$$mv^2 r = 5.7926 \frac{e^2}{4\pi\varepsilon_o}$$

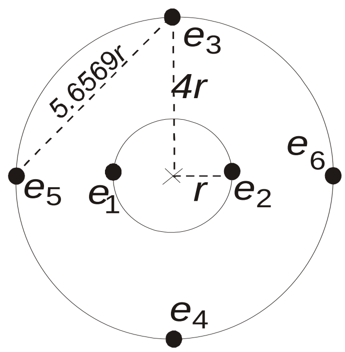

Figure 4 - Carbon neutral atom with 6 electrons

From Section 1.2 for e_1 and e_2 is:

$$V_{qu.1.e} = \frac{e^2}{4\pi\varepsilon_o}\left(\frac{6}{r} - \frac{1}{2r} - \frac{1}{5r} - \frac{1}{3r} - \frac{2}{4.1231r}\right) = 4.4815\frac{e^2}{4\pi\varepsilon_o}\frac{1}{r}$$

From section 1.3 we have:

$$V_{m.e1} = V_{m.e2} = -\frac{Ze^2}{4\pi\varepsilon_o r} = -\frac{e^2}{4\pi\varepsilon_o}\frac{6}{r}$$

Making the same sequence of calculation of the electrons 1 and 2 of He we have

$$r = 0.28842\frac{4\pi\varepsilon_o}{e^2}\frac{n^2\hbar^2}{m} \qquad (36)$$

$$K_{e1} = K_{e2} = \frac{1}{2}20.083\frac{e^4}{(4\pi\varepsilon_o)^2}\frac{m}{n^2\hbar^2}$$

$$V_{m.e1} = V_{m.e2} = -20.803\frac{e^4}{(4\pi\varepsilon_o)^2}\frac{m}{n^2\hbar^2}$$

6.2 – Electron 3 and 4

The modified potencial energy for e3 and e4 is:

$$V_{m.e3} = V_{m.e4} = \frac{V_{m.1e}}{n^2} = \frac{V_{m.1e}}{4} = -5.2007\frac{e^4}{(4\pi\varepsilon_o)^2}\frac{m}{\hbar^2}$$

The forces are:

$$m\frac{v^2}{4r}=\frac{e^2}{4\pi\varepsilon_o}\left(\frac{6}{(4r)^2}-\frac{1}{(8r)^2}-\frac{2\cos 14.036}{\left(4.1231r^2\right)}-\frac{2sin45}{(5.6568r)^2}\right)$$

$$mv^2r=0.8042\frac{e^2}{4\pi\varepsilon_o} \qquad (37)$$

Substituting (36) in (37) we have:

$$v^2=2.7883\frac{e^4}{(4\pi\varepsilon_o)^2}\frac{1}{n^2\hbar^2}$$

$$K_{e3}=K_{e4}=\frac{1}{2}2.7883\frac{e^4}{(4\pi\varepsilon_o)^2}\frac{m}{n^2\hbar^2}$$

6.3 – Electron 5 and 6

The modified potencial energy for e5 and e6 is:

$$V_{m.e5}=V_{m.e6}=\frac{V_{m.1e}}{n^2}=\frac{V_{m.1e}}{4}=-5.2007\frac{e^4}{(4\pi\varepsilon_o)^2}\frac{m}{\hbar^2}$$

The forces are:

$$m\frac{v^2}{4r}=\frac{e^2}{4\pi\varepsilon_o}\left(\frac{6}{(4r)^2}-\frac{1}{(3r)^2}-\frac{1}{(8r)^2}-\frac{2sin45}{(5.6568r)^2}\right)$$

$$mv^2r=0.81628\frac{e^2}{4\pi\varepsilon_o} \qquad (38)$$

Substituting (36) in (38) we have:

$$v^2=2.8302\frac{e^4}{(4\pi\varepsilon_o)^2}\frac{1}{n^2\hbar^2}$$

$$K_{e5}=K_{e6}=\frac{1}{2}2.8302\frac{e^4}{(4\pi\varepsilon_o)^2}\frac{m}{n^2\hbar^2}$$

The total energy of the C I is:

$$E = K_{e1} + K_{e2} + K_{e3} + K_{e4} + K_{e5} + K_{e6} + V_{m.e1} + V_{m.e2} + V_{m.e3} + V_{m.e4} + V_{m.e5} + V_{m.e6}$$

$$E = 2(10.042 + 1.3941 + 1.4151) - 2(20.803 + 5.2007 + 5.2007)27.2 = -998.4 \text{ eV}$$

7. Relativistic correction

Consider the Fm C (one electron, Z=100), and the velocity is 0.7333c.
We make an approach and consider the electron with circular path and the forces are:

$$\frac{m_o}{\sqrt{1-\beta^2}} \frac{v^2}{r} = \frac{e^2}{4\pi\varepsilon_o} \frac{100}{r^2}$$

The relativistic kinetic energy is:

$$K_e = m_o c^2 \left(\frac{1}{\sqrt{1-\beta^2}} - 1 \right)$$

The equation above are the relativistic correction.
Making the calculations with the equations above we have the results presented in the tables 1, 2 and 3.

	Z	e-	β	r (relat.)	E (Newt.)	E (relat.)
				x10^{-11}m	error %	error %
H I	1	1	0.0073	5.29	0.0	0.0
He II	2	1	0.0147	2.65	0.0	0.0
C VI	6	1	0.0440	0.88	0.1	0.0
P XV	15	1	0.1100	0.35	-0.3	0.0
Ca XX	20	1	0.1467	0.26	-0.5	0.0
Zn XXX	30	1	0.2200	0.17	-1.2	0.0
Sn L	50	1	0.3667	0.098	-3.4	0.1
Hg LXXX	80	1	0.5866	0.053	-9.2	0.3
Fm C	100	1	0.7333	0.036	-15.2	0.6

Table 3 - . Error in % between the atom energy theoretical and experimental. Energy calculated with Newtonian equations and with relativistic correction.

Conclusion

This method of calculation of the atoms energy levels has the maximum error of 3.6%.
In this paper we use only the Coulomb force. And it is necessary to continue the research and to include the other forces.

References

[1] NIST Atomic Spectra Database Ionization Energies Data: binding energy. http://physics.nist.gov/PhysRefData/ASD/ionEnergy.html