Atomic excited states and the related energy levels

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Research Article

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Atomic excited states and the related energy levels⊗

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Abstract:
The general theory of atoms including the related excited states and energy levels is reviewed. Numerical calculations and detailed works for several elements are presented to establish a better understanding of excited states. The article seeks also for connections between atomic behavior, and the internal structures and inner electrons of atoms. Then the atomic excited energy levels are formulated using the corresponding atomic ionization energies and a new defined parameter called "Characteristic exponent k". Furthermore, a small data bank is generated using the calculated "characteristic exponents k" for elements to be utilized for future simulations, studies, research activities and a connection to the type of atoms and their internal atomic structures.

Keywords: Excited States, Atomic Energy Levels, Classical Energy Model, Simulated Energy Model, Ionization Energy, Characteristic Exponent k, Bohr's Perception, De Broglie's View

Introduction:
The primary objective of this article is to introduce a simple approach to estimate excited energy levels of atoms. The article is a continuation of a few earlier works [1-4] as well as the previous research activities [5-6] to establish a better understanding of atomic and molecular structures and the related energies. To achieve the goal of this article, a quick review of earlier concepts and theories seems to be necessary. Thus a review over the classical theory of motion, atomic energy, and the concept of excited states is made before presenting the results.

Classical energy model and concepts [7-16]
In 1924, a French physicist **Louis de Broglie** postulated a new concept that all moving objects have a wave-like motion with an associated wavelength. The concept is known as wave-particle duality which forms the foundation of quantum mechanics. According to his postulate the wavelength of any moving object is inversely proportional to the linear momentum of the object (Eq.1).

$$\lambda = \frac{h}{mv} \qquad (1)$$

where λ is the wavelength of object, h the Plank's constant, m the mass, and v the velocity of object. Figure 1 presents the De Broglie's perception for motion of different objects. According to his concept, an electron with a mass of 9.109534E-31 kg moving

with 1/10 of speed of light around nucleus would have a wavelength of 2.42E-11 meter. A baseball with 5 ounce mass thrown by the baseball pitcher, Nolan Ryan in 1974 with a speed of 100.9 mph would have a wavelength of 1.036E-34 m. And finally the planet earth with a mass of 5.972E24 kg and a speed of 30 km/s around the sun would have a wavelength of 3.698E-63 m. Hence in brief, smaller objects with common speeds would have larger wavelengths compared to larger objects.

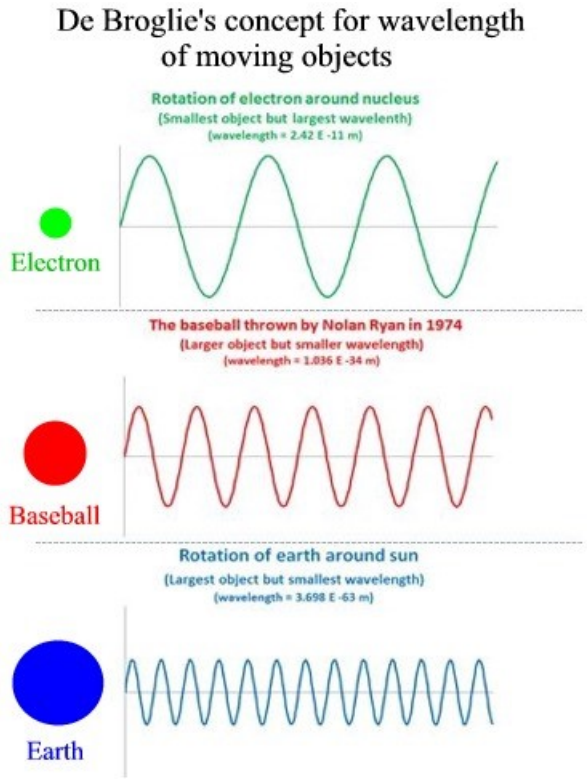

Figure 1: De Broglie's postulate of moving objects.

In 1913, **Niels Bohr** and **Ernest Rutherford** presented their atomic model as a model for **one-electron atom** (i.e. Hydrogen). The concept assumed circular orbit for the electron in equilibrium under two forces. One force was the centripetal force acting on the electron due to its rotational speed which was assumed to be equal to the attracting coulombic force acting on electron by the nucleus (Eq.2).

$$\frac{m_e v^2}{r} = \frac{Ze^2}{r^2} \tag{2}$$

where m_e is the mass of electron, v the velocity of electron, r the orbital radius, Z the atomic number, and e the electron's charge, all in atomic units. To assure that the electron would stay in a certain orbits consistent with common observations and the notion of ground and excited state energy levels, Bohr needed to make an additional assumption. He postulated that the circumference (/radius) of the electronic path should be able to accommodate a whole number of electronic wavelength to assure separate electronic orbits as well as different vibrational modes for both ground (n = 1) and excited states (n

= 2, 3, 4, …). This way, he tied the atomic excitation states to vibrational modes of electron.

$$2\pi r = n\,\lambda \tag{3}$$

where r is the electronic radius, n the number of excited state (or vibrational mode) and λ the wavelength of moving electron. Figure 2 presents the Bohr's view of electronic orbits in ground and excited states of hydrogen.

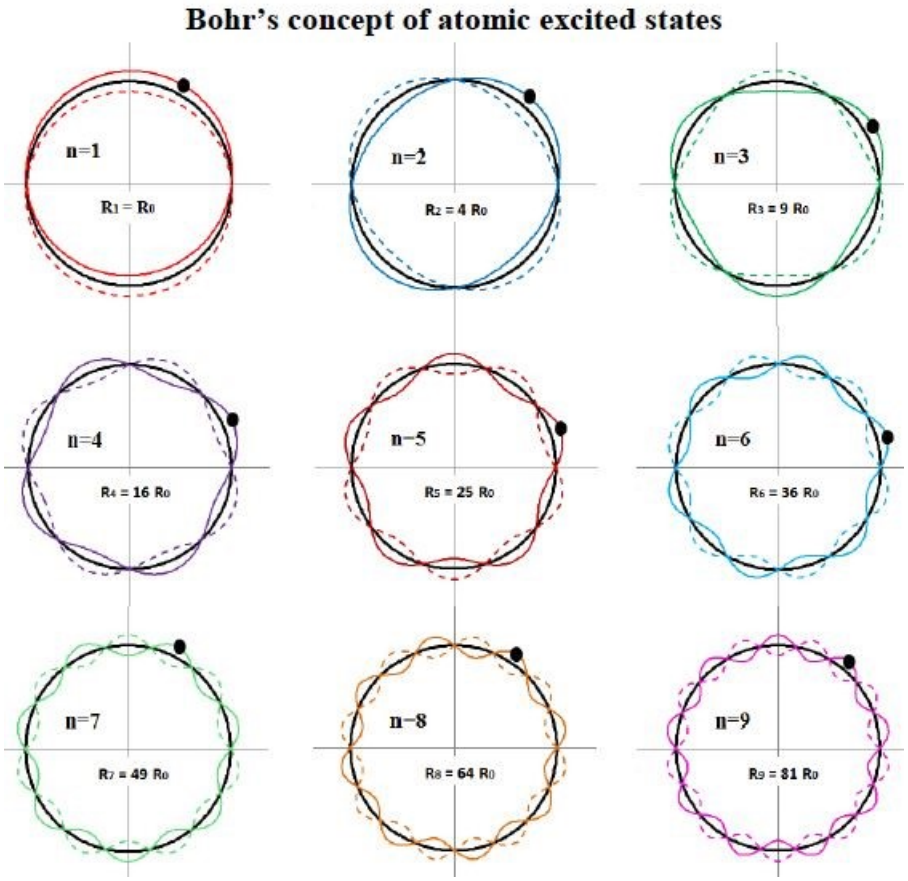

Figure 2: Bohr's view of atomic excitation states for Hydrogen

Hence the concept of excited state could be viewed as electronic vibrational mode. The theory needed one more component which was the **Planck**'s formula (or Plank's energy-frequency relationship) which is presented by Eq.4.

$$\Delta E = h\,\vartheta \tag{4}$$

where ΔE is the energy change, h is the Plank's coefficient and ϑ presents the frequency. Combining Eq.1 and Eq.3, one can derive Eq.5 which relates the rotational momentum (mvr) to the excitation state or vibrational mode n as:

$$mvr = n(h/2\pi) \tag{5}$$

Then the Eq.6 can be derived by the rearrangement of Eq.2 as:

$$r = \frac{Ze^2}{m_e v^2} \tag{6}$$

Furthermore, combining Eq. 2, 5 & 6, one can obtain an equation for the ground state and excited states radii (Eq. 7) as:

$$R_n = \left[\frac{(h/2\pi)^2}{Z \cdot m_e \cdot e^2}\right] \cdot n^2 = R_0 \cdot n^2 \tag{7}$$

where R_0 is the ground state electronic radius for one-electron atom, R_n the electronic radius in excited states and n is the number of excited state or the vibrational mode. n can take only whole numbers representing different excited states. Using the formal classical mechanics, then one can write Eq.8 for the kinetic energy of the electron and Eq.9 for the potential energy of interaction between electron and nucleus as:

$$E_k = Kinetic\ Energy = +\,{}^1\!/_2\, m_e v^2 \tag{8}$$

$$E_p = Potential\ Energy = -\frac{Ze^2}{r} \tag{9}$$

But the magnitude of potential energy (E_p) is twice of the kinetic energy (E_k). And hence the total energy of the one-electron system can be written as summation of those two energies as presented by (Eq.10) in atomic units:

$$E_{tot} = E_{G.S.} = Total\ Energy = E_k + E_p = -\frac{Ze^2}{2r} = -\,{}^1\!/_2\, m_e v^2 \tag{10}$$

Combining Eq. 2 & 5, one can easily conclude that velocity of the electron in excited states would be inversely proportional to the n which is the related number for excited state and vibrational mode. This would provide a new equation (Eq.11) for the total energy of the one-electron model in ground and excited state modes (E_n) as:

$$E_n = -\left[\frac{Z \cdot e^2}{2R_0}\right] \cdot \left(\frac{1}{n^2}\right) = E_0 \cdot \left(\frac{1}{n^2}\right) = E_{G.S.} \cdot \left(\frac{1}{n^2}\right) \tag{11}$$

But we know that the total energy of one-electron atom in ground state is equal to its related ionization energy (Eq.12) which can be found experimentally. Therefore,

$$E_{tot} = E_{G.S.} = Ionization\ Energy = E_{ioniz} \tag{12}$$

Now we are ready to expand our theory to multi-electron atoms by making minor changes to our classical atomic energy theory. What we know that having inner electrons in the model would only impact the Eq.2. Figure 3 presents the case of multi-electron case.

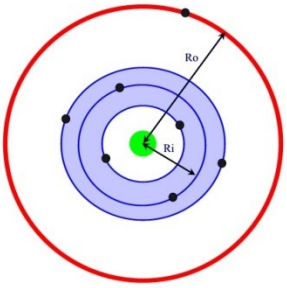

Figure 3: Schematic diagram of multi-electron atoms

As one can observe in the Figure 3, the outer electron in multi-electron atoms would be subjected to two forces and would be interacting not only with the nucleus at R_o radius but also would be interacting with inner electrons which are at R_i radii. The existence of inner electrons will transform Eq.2 to a new form shown as Eq.13 where the impact of inner electrons on the force balance equation can be approximated by:

$$\frac{m_e v^2}{r_o} = \frac{Ze^2}{{r_o}^2} - \sum \frac{e^2}{(\boldsymbol{r}_o - \boldsymbol{r}_i)^2} \tag{13}$$

in which $\mathbf{r}_o$ and $\mathbf{r}_i$ are vectors and the summation terms are projected in radial direction. The existence of inner electrons brings in more complexity, randomness and nonlinearity to the governing equations and the **exponent 2** for the n which is the number of excited state in our classical model would now be changing to a different number between 0 and 2 such as 0.92 for Rubidium. We will be calling this new parameter "characteristic exponent k" for the rest of this article.

Therefore, our governing equations would look more like Eq.14 and Eq.15 in which the exponents 2 are replaced by k which would be a number less than 2 depending on the inner electronic structure of atom. The k factor will be equal to 2 only for hydrogen and would have different values for the rest of atoms which would be needed to be determined.

Hence **Characteristic Exponent k** is the exponent of n in our updated model and is a parameter which would provide us information about the inner structure of atoms. Also the characteristic exponent k of an atom would help us to determine all excited state energy levels of the each atom or ion. The characteristic exponent k of several elements are found and presented at the end of this article.

$$R_n = \left[\frac{(h/2\pi)^2}{Z \cdot m_e \cdot e^2}\right] \cdot n^{\boldsymbol{k}} = R_0 \cdot n^{\boldsymbol{k}} \tag{14}$$

$$E_n = -\left[\frac{Z \cdot e^2}{2R_0}\right] \cdot \left(\frac{1}{n^{\boldsymbol{k}}}\right) = E_0 \cdot \left(\frac{1}{n^{\boldsymbol{k}}}\right) = E_{G.S.} \cdot \left(\frac{1}{n^{\boldsymbol{k}}}\right) \tag{15}$$

To better understand the case, let's summarize the author's conclusion from his observations. Readers would check all of the points for themselves in upcoming figures and discussions.

1. During the excitation of atoms only one electron which is the one furthest away from nucleus would move away into excited states.
2. Analogy of a closed chest with one opening for only one electron at the time to move out applies to all of the inner electrons of the atoms. All inner electrons are kept in place as the outer electron goes through the excitation.
3. If an outer electron leaves away from the atom, then a new electron will be able to move out and fill the excited states. But now the atom would turn to a positively charged ion with a new ionization energy (or $E_{G.S.}$).
4. In all possible excitation cases, there would be only one electron at the time going through the excitation and only one ionization energy figure would govern the excited energy levels.
5. The two factors governing the excited energy levels would be the ionization energy of the specie and the related excited state or vibrational mode of the electron.
6. Hence the equation of $E_n=(I.E.)/n^k$ can be used to find all excited energy levels as long as k and I.E. are known.

Methodology:

To find the characteristic exponents k of atoms, the author needed all experimental ionization energies as well as the experimental energy levels of atoms and ions. These data have been experimentally measured throughout years by different researchers and the collected measured values are available through different sources [17-20]. But one of the best reliable sources of experimental data for our purpose is the online NIST Database website [17] which provides reliable "atomic spectra energy level and ionization energy" values. NIST stands for the National Institute of Standards and Technology and is a governmental institute which collects and maintains reliable experimental data for research and industrial use. All available experimental energy values of atoms and ions were downloaded and collected from NIST websites for being used in this article.

But it needs to be told that the downloaded energy level data from NIST websites were loaded with all sorts of notations, configurations, splitting and maybe with some multiplicities, duplications and degeneracies which made it real hard for the author to identify and separate the actual individual atomic energy levels of the excited states. Hence the author had to resort to the concept that actual reported energy values for excited states should be consistent in their magnitudes within the arbitrary figure of 0.01 eV for each energy level and therefore all reported energy values within 0.01 eV should be actually originated from the same root and should not be considered as separate energy levels. This remedy generally condensed the huge number of energy levels to a manageable level below 100. In some occasions, the reported energy values within 0.05 eV were considered having a common root and were considered to be one energy level.

Results:

Results and graphs are presented for a few selected atoms in the article while all of the collected data, results and graphs are shown in the "Supplementary Data" for the readers to review. We will start with hydrogen atom.

Hydrogen (H)

The one-electron hydrogen is the basis for our classical theory. The atom does not have any inner electron and therefore it is completely consistent with our theoretical model. Figure 4 presents both tabulated and graphical displays of the energy levels for the atom. As one can observe, the experimental figures are completely in line with our classical model which gives credibility to the approach. Errors are zero and the experimental data fall all on the simulated graph. This atom belongs to group 1 (IA) of s block.

Hydrogen (H) Ionization Energy, I.E.(1st) = -13.6 eV Characteristic exponent k = 2			
Axis	Experimental energy levels (eV)	Classical energy Model (eV)	Absolute Error (eV)
1	-13.60	-13.60	0.00
2	-3.40	-3.40	0.00
3	-1.51	-1.51	0.00
4	-0.85	-0.85	0.00
5	-0.55	-0.54	0.00
6	-0.38	-0.38	0.00
7	-0.28	-0.28	0.00
8	-0.21	-0.21	0.00
9	-0.17	-0.17	0.00
10	-0.14	-0.14	0.00

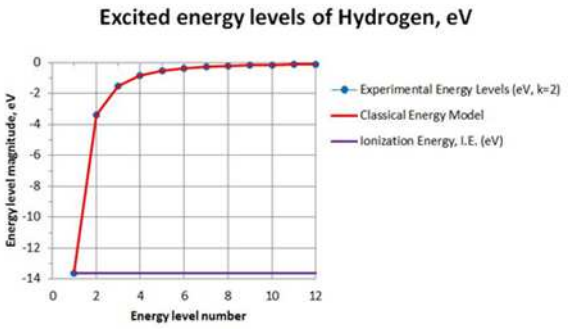

Figure 4: Tabulated and graphical presentation of energy levels of Hydrogen

Helium (He I)

Helium atom has two electrons with one to be considered an inner electron for the other outer electron. So the atom is not completely in line with our classical model due to the inner electron. Figure 5 presents both tabulated and graphical displays of the energy levels for this atom. As one can observe, the experimental figures are not completely in line with our classical model. This is due to the inner electron and a departure of 2 to 1.35 happens to the characteristic exponent k of this atom to bring the simulated graph closer to the experimental data. An average of 0.28 eV absolute error was observed for this atom. This atom belongs to group 18 (O) of s-block.

Helium (He I) Ionization Energy, I.E.(1st) = -24.6 eV Characteristic exponent k = 1.35				
Axis	Experimental energy levels (eV)	Simulated energy levels (eV, k=1.35)	Classical energy model (H) (eV)	Absolute error, eV
1	-24.60	-24.60	-24.60	0.00
2	-4.78	-9.65	-6.15	4.87
3	-3.98	-5.58	-2.73	1.60
4	-3.64	-3.79	-1.54	0.15
5	-3.38	-2.80	-0.98	0.58
6	-1.88	-2.19	-0.68	0.31
7	-1.68	-1.78	-0.50	0.10
8	-1.59	-1.49	-0.38	0.11
9	-1.53	-1.27	-0.30	0.26
10	-1.51	-1.10	-0.25	0.41

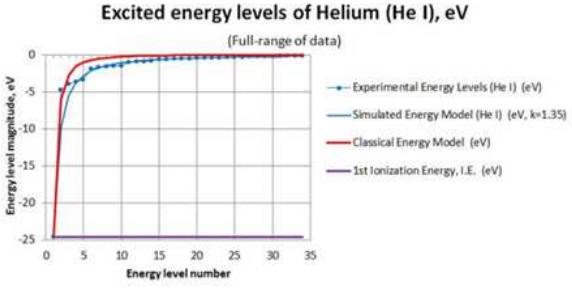

Figure 5: Tabulated and graphical presentation of energy levels of Helium

Lithium (Li I)

Lithium atom has three electrons with two to be considered inner electrons for the outer electron. So the atom is not in line with our classical model due to the inner electrons. Figure 6 presents both tabulated and graphical displays of the energy levels for this atom. As one can observe, the experimental figures are not in line with our classical model. This is due to the inner electrons and a departure of 2 to 0.96 happens to the characteristic exponent k of this atom to bring the simulated graph closer to the experimental data. An average absolute error value of 0.14 eV was observed for this atom. This atom belongs to group 1 (IA) of s-block.

Lithium (Li I) Ionization Energy, I.E.(1st) = -5.4 eV Characteristic exponent k = 0.96				
Axis	Experimental energy levels (Li I) (eV)	Simulated energy levels (Li I) (eV, k=0.96)	Classical energy levels (H) (eV)	Absolute error, eV
1	-5.40	-5.40	-5.40	0.00
2	-3.55	-2.78	-1.35	0.78
3	-2.03	-1.88	-0.60	0.15
4	-1.57	-1.43	-0.34	0.14
5	-1.52	-1.15	-0.22	0.37
6	-1.06	-0.97	-0.15	0.09
7	-0.88	-0.83	-0.11	0.04
8	-0.86	-0.73	-0.08	0.12
9	-0.65	-0.66	-0.07	0.00
10	-0.56	-0.59	-0.05	0.03

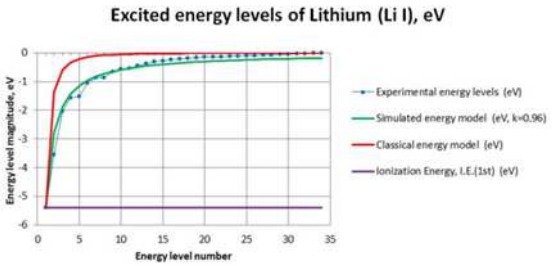

Figure 6: Tabulated and graphical presentation of energy levels of Lithium

Beryllium (Be I, II, III, IV):

Beryllium atom has four electrons with three to be considered inner electrons for the outer electron. So the atom is not in line with our classical model due to the inner electrons. Figure 7 presents the graphical displays of the energy levels for this atom and its ions. As one can observe, none of the experimental data are in line with our classical model. This is due to the inner electrons and a departure of 2 to 1.75 for Be IV, a departure of 2 to 1.13 for Be III, a departure of 2 to 0.93 for Be II and a departure of 2 to 0.79 for Be I happens to the characteristic exponent k of this atom and its ions to adjust the simulated graphs closer to the experimental data. Average absolute error values of 0.16 eV for Be I, 0.57 eV for Be II, 3.28 eV for Be III and 2.29 eV for Be IV were observed for this atom and its ions. This atom belongs to group 2 (IIA) of s-block.

Now it is important to make some conclusions about the excited states using our observations of this atom and its ions. First we can see that each specie uses its own outer ionization energy to establish its excited energy levels which means Be I uses $E_n=(9.323)/n^{0.79}$, Be II uses $E_n=(18.211)/n^{0.93}$, Be III uses $E_n=(153.896)/n^{1.13}$ and Be IV uses $E_n=(217.718)/n^{1.75}$ to establish the energy levels. This proves some sort of independency among the ions which would indicate that the inner electrons are not affected by an outer electron in excitation mode. As a reminder, the equation of $E_n=(I.E.)/n^k$ is always used to simulate the excited energy levels of each specie.

Second, if the inner electrons were disturbed by the excitation of outer electron, then this would have affected the ionization energy of the excited electron which is not the case. The excited energy levels are only governed by fixed ionization energy throughout the excitation. If there was not an independency with respect to the inner electrons, then we should have also seen that the ionization energy figures of other ionic species affecting

the energy levels of targeted specie. In other words $(I.E.)_2$ of Be II, and $(I.E.)_3$ of Be III and $(I.E.)_4$ of Be IV should have also played a role and must have affected the energy levels of Be I due to lack of independency which is not observed.

So during the excitation of atoms/ions only one electron which is the one furthest away from nucleus would move away into excited states and the analogy of a closed chest with one opening for only one electron at the time to move out should apply to inner electrons of atoms. Hence all inner electrons must been have kept in place as the outer electron goes through the excitation. And if an outer electron leaves the atom, then a new electron will be able to move out and fill the excited states. But in all possible ions of an atom, there would be only one electron at the time going through the excitation and only one ionization energy figure would govern the excited energy levels of that specie.

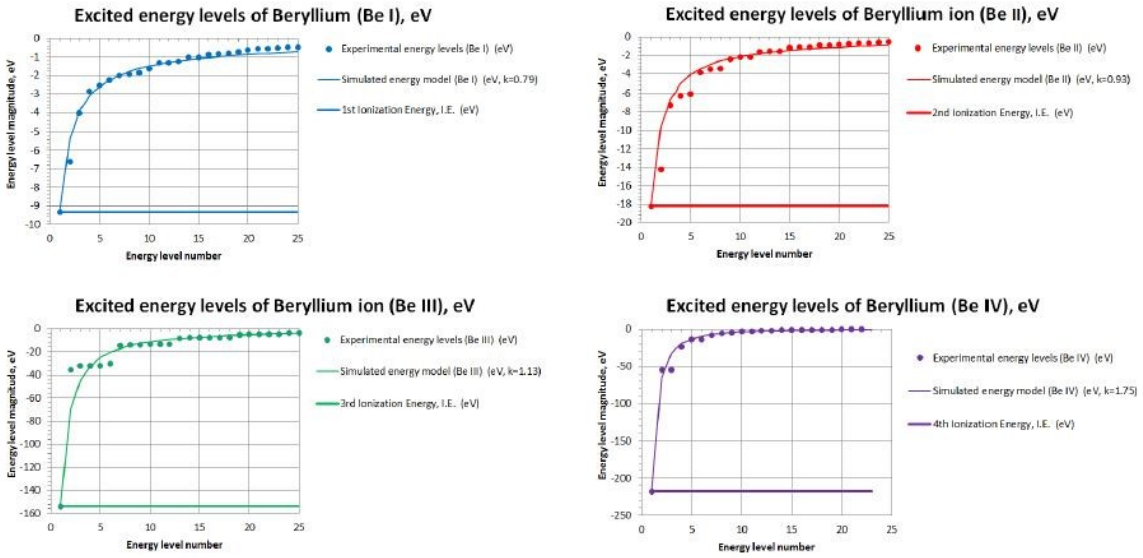

Figure 7: Graphical presentation of energy levels of Beryllium atom and its ions

Boron (B I)

Boron atom has five electrons with four to be considered inner electrons for the outer electron. So the atom is not in line with our classical model due to the inner electrons. Figure 8 presents the graphical display of energy levels for this atom. As one can observe, the experimental figures are not in line with our classical model. This is due to the inner electrons and a departure of 2 to 1.10 happens to the characteristic exponent k of this atom to bring the simulated graph closer to the experimental data. An average absolute error value of 0.21 eV was observed for this atom. This atom belongs to group 13 (IIIA) of p-block.

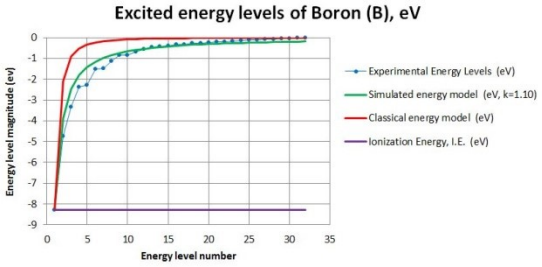

Figure 8: Graphical presentation of energy levels of Boron

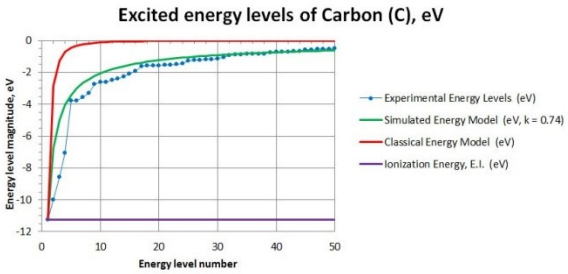

Figure 9: Graphical presentation of energy levels of Carbon

Carbon (C I)

Carbon atom has six electrons with five to be considered inner electrons for the outer electron. So the atom is not in line with our classical model due to the inner electrons. Figure 9 presents the graphical display of energy levels for this atom. Due to the inner electrons, a departure of 2 to 0.74 happens to the characteristic exponent k of this atom to bring the simulated graph closer to the experimental data. An average absolute error value of 0.38 eV was observed for this atom. This atom belongs to group 14 (IVA) of p-block.

Nitrogen (N I)

Nitrogen atom has seven electrons with six to be considered inner electrons for the outer electron. So the atom is not in line with our classical model due to the inner electrons. Figure 10 presents the graphical display of energy levels for this atom. Due to the inner electrons, a departure of 2 to 0.57 happens to the characteristic exponent k of this atom to bring the simulated graph closer to the experimental data. An average absolute error value of 0.26 eV was observed for this atom. This atom belongs to group 15 (VA) of p-block.

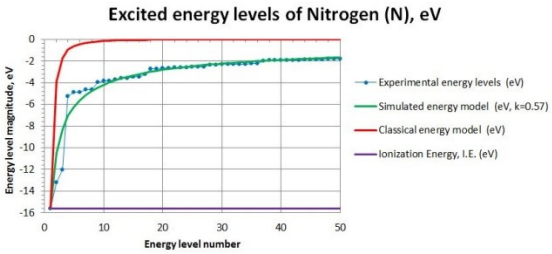

Figure 10: Graphical presentation of energy levels of Nitrogen

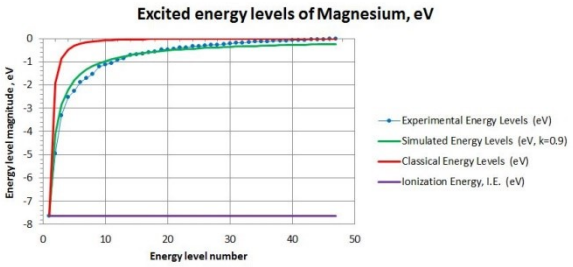

Figure 11: Graphical presentation of energy levels of Magnesium

Magnesium (Mg I)

Magnesium atom has 12 electrons with 11 to be considered inner electrons for the outer electron. So the atom is not in line with our classical model due to the inner electrons. Figure 11 presents the graphical display of energy levels for this atom. Due to the inner electrons, a departure of 2 to 0.9 happens to the characteristic exponent k of this atom to bring the simulated graph closer to the experimental data. An average absolute error value of 0.18 eV was observed for this atom. This atom belongs to group 2 (IIA) of s-block.

Aluminum (Al I)

Aluminum atom has 13 electrons with 12 to be considered inner electrons for the outer electron. So the atom is not in line with our classical model due to the inner electrons. Figure 12 presents the graphical display of energy levels for this atom. Due to the inner electrons, a departure of 2 to 0.85 happens to the characteristic exponent k of this atom to bring the simulated graph closer to the experimental data. An average absolute error value of 0.05 eV was observed for this atom. This atom belongs to group 13 (IIIA) of p-block.

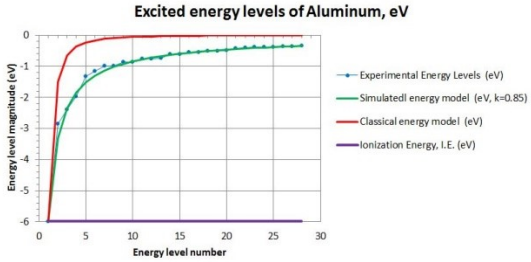

Figure 12: Graphical presentation of energy levels of Aluminum

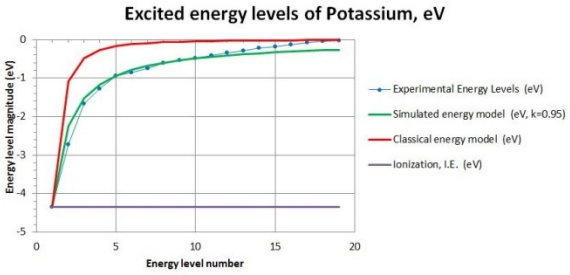

Figure 13: Graphical presentation of energy levels of Potassium

Potassium (K I)

Potassium atom has 19 electrons with 18 to be considered inner electrons for the outer electron. So the atom is not in line with our classical model due to the inner electrons. Figure 13 presents the graphical display of energy levels for this atom. Due to the inner electrons, a departure of 2 to 0.95 happens to the characteristic exponent k of this atom to bring the simulated graph closer to the experimental data. An average absolute error value of 0.12 eV was observed for this atom. This atom belongs to group 1 (IA) of s-block.

Nickel (Ni I)

Nickel atom has 28 electrons with 27 to be considered inner electrons for the outer electron. So the atom is not in line with our classical model due to the inner electrons. Figure 14 presents the graphical display of energy levels for this atom. Due to the inner electrons, a departure of 2 to 0.35 happens to the characteristic exponent k of this atom to bring the simulated graph closer to the experimental data. An average absolute error value of 1.05 eV was observed for this atom. This atom belongs to group 10 (VIII) of d-block.

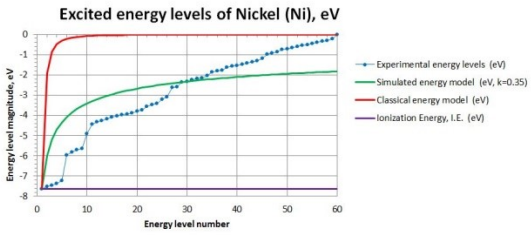

Figure 14: Graphical presentation of energy levels of Nickel

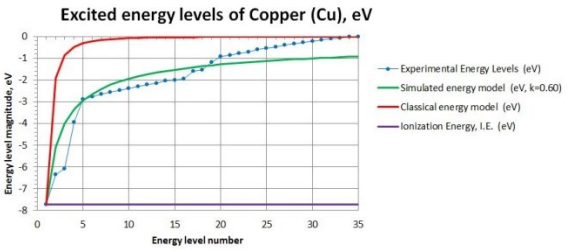

Figure 15: Graphical presentation of energy levels of Copper

Copper (Cu I)

Copper atom has 29 electrons with 28 to be considered inner electrons for the outer electron. So the atom is not in line with our classical model due to the inner electrons. Figure 15 presents the graphical display of energy levels for this atom. Due to the inner electrons, a departure of 2 to 0.6 happens to the characteristic exponent k of this atom to bring the simulated graph closer to the experimental data. An average absolute error value of 0.56 eV was observed for this atom. This atom belongs to group 11 (IB) of d-block.

Zinc (Zn I)

Zinc atom has 30 electrons with 29 to be considered inner electrons for the outer electron. So the atom is not in line with our classical model due to the inner electrons. Figure 16 presents the graphical display of energy levels for this atom. Due to the inner electrons, a departure of 2 to 0.91 happens to the characteristic exponent k of this atom to bring the simulated graph closer to the experimental data. An average absolute error value of 0.37 eV was observed for this atom. This atom belongs to group 12 (IIB) of d-block.

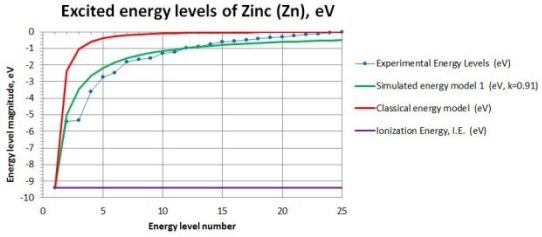

Figure 16: Graphical presentation of energy levels of Zinc

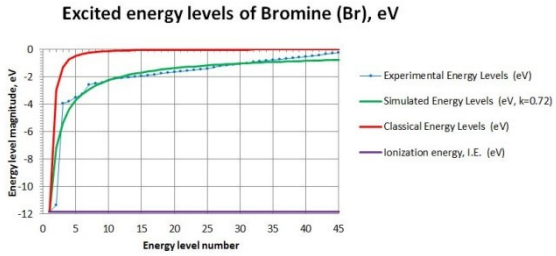

Figure 17: Graphical presentation of energy levels of Bromine

Bromine (Br I)

Bromine atom has 35 electrons with 34 to be considered inner electrons for the outer electron. So the atom is not in line with our classical model due to the inner electrons. Figure 17 presents the graphical display of energy levels for this atom. Due to the inner electrons, a departure of 2 to 0.72 happens to the characteristic exponent k of this atom to bring the simulated graph closer to the experimental data. An average absolute error value of 0.35 eV was observed for this atom. This atom belongs to group 17 (VIIA) of p-block.

Krypton (Kr I)

Krypton atom has 36 electrons with 35 to be considered inner electrons for the outer electron. So the atom is not in line with our classical model due to the inner electrons. Figure 18 presents the graphical display of energy levels for this atom. Due to the inner electrons, a departure of 2 to 0.92 happens to the characteristic exponent k of this atom to bring the simulated graph closer to the experimental data. An average absolute error value of 0.35 eV was observed for this atom. This atom belongs to group 18 (O) of p-block.

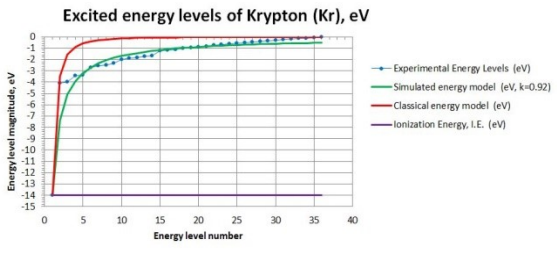

Figure 18: Graphical presentation of energy levels of Krypton

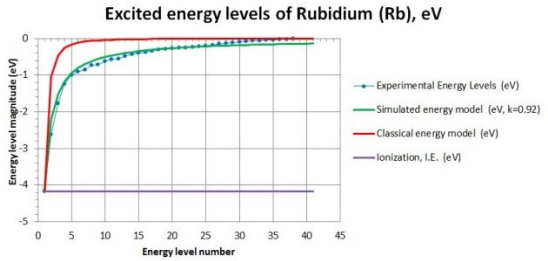

Figure 19: Graphical presentation of energy levels of Rubidium

Rubidium (Rb I)

Rubidium atom has 37 electrons with 36 to be considered inner electrons for the outer electron. So the atom is not in line with our classical model due to the inner electrons. Figure 19 presents the graphical display of energy levels for this atom. Due to the inner electrons, a departure of 2 to 0.92 happens to the characteristic exponent k of this atom to bring the simulated graph closer to the experimental data. An average absolute error value of 0.09 eV was observed for this atom. This atom belongs to group 1 (IA) of s-block.

Molybdenum (Mo I)

Molybdenum atom has 42 electrons with 41 to be considered inner electrons for the outer electron. So the atom is not in line with our classical model due to the inner electrons. Figure 20 presents the graphical display of energy levels for this atom. Due to the inner electrons, a departure of 2 to 0.17 happens to the characteristic exponent k of this atom to bring the simulated graph closer to the experimental data. An average absolute error value of 0.12 eV was observed for this atom. This atom belongs to group 6 (VIB) of d-block.

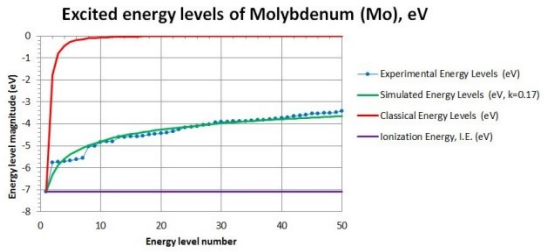

Figure 20: Graphical presentation of energy levels of Molybdenum

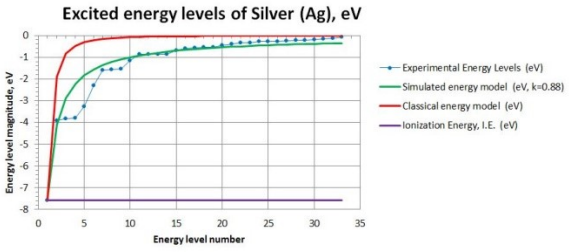

Figure 21: Graphical presentation of energy levels of Silver

Silver (Ag I)

Silver atom has 47 electrons with 46 to be considered inner electrons for the outer electron. So the atom is not in line with our classical model due to the inner electrons. Figure 21 presents the graphical display of energy levels for this atom. Due to the inner electrons, a departure of 2 to 0.88 happens to the characteristic exponent k of this atom to bring the simulated graph closer to the experimental data. An average absolute error value of 0.27 eV was observed for this atom. This atom belongs to group 11 (IB) of d-block.

Iodine (I I)

Iodine atom has 53 electrons with 52 to be considered inner electrons for the outer electron. So the atom is not in line with our classical model due to the inner electrons. Figure 22 presents the graphical display of energy levels for this atom. Due to the inner electrons, a departure of 2 to 0.6 happens to the characteristic exponent k of this atom to bring the simulated graph closer to the experimental data. An average absolute error value of 0.22 eV was observed for this atom. This atom belongs to group 17 (VIIA) of p-block.

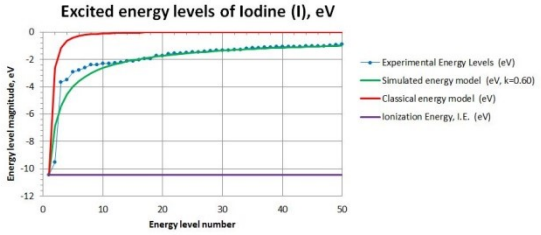

Figure 22: Graphical presentation of energy levels of Iodine

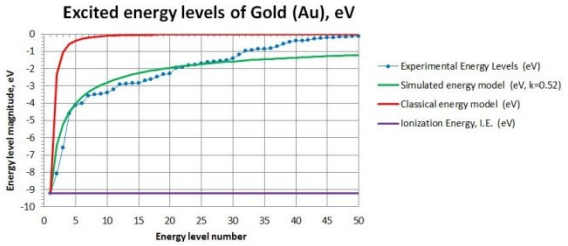

Figure 23: Graphical presentation of energy levels of Gold

Gold (Au I)

Gold atom has 79 electrons with 78 to be considered inner electrons for the outer electron. So the atom is not in line with our classical model due to the inner electrons. Figure 23 presents the graphical display of energy levels for this atom. Due to the inner electrons, a departure of 2 to 0.52 happens to the characteristic exponent k of this atom to bring the simulated graph closer to the experimental data. An average absolute error value of 0.55 eV was observed for this atom. This atom belongs to group 11 (IB) of d-block.

Mercury (Hg I)

Mercury atom has 80 electrons with 79 to be considered inner electrons for the outer electron. So the atom is not in line with our classical model due to the inner electrons. Figure 24 presents the graphical display of energy levels for this atom. Due to the inner electrons, a departure of 2 to 0.83 happens to the characteristic exponent k of this atom to bring the simulated graph closer to the experimental data. An average absolute error value of 0.23 eV was observed for this atom. This atom belongs to group 12 (IIB) of d-block.

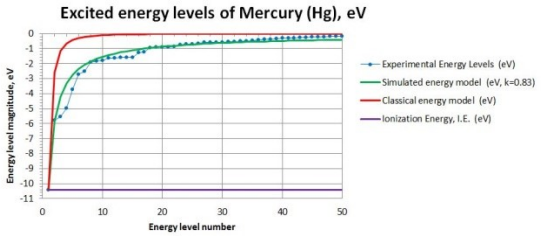

Figure 24: Graphical presentation of energy levels of Mercury

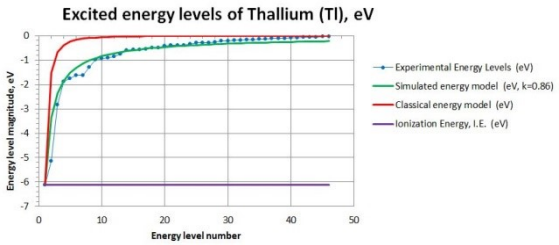

Figure 25: Graphical presentation of energy levels of Thallium

Thallium (Tl I)

Thallium atom has 81 electrons with 80 to be considered inner electrons for the outer electron. So the atom is not in line with our classical model due to the inner electrons. Figure 25 presents the graphical display of energy levels for this atom. Due to the inner electrons, a departure of 2 to 0.86 happens to the characteristic exponent k of this atom to bring the simulated graph closer to the experimental data. An average absolute error value of 0.16 eV was observed for this atom. This atom belongs to group 13 (IIIA) of p-block.

Francium (Fr I)

Francium atom has 87 electrons with 86 to be considered inner electrons for the outer electron. So the atom is not in line with our classical model due to the inner electrons. Figure 26 presents the graphical display of energy levels for this atom. Due to the inner electrons, a departure of 2 to 0.77 happens to the characteristic exponent k of this atom to bring the simulated graph closer to the experimental data. An average absolute error value of 0.18 eV was observed for this atom. This atom belongs to group 1 (IA) of s-block.

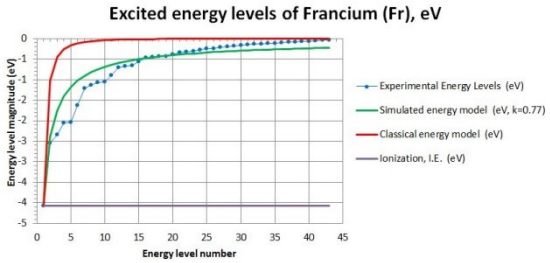

Figure 26: Graphical presentation of energy levels of Francium

Tabulation and Analysis of Collected Results:

Figure 27, Figure 28 and Table 1 present variations of characteristic exponent k among the elements of periodic table. Figure 27 shows the variation of k value in segmented rows of periodic table. Each segment/row has been shown with a different color for clarity. Figure 28 presents the variation of characteristic exponent k for different groups of atoms such as s-block (H & He), s-block (G1, G2), p-block (G13-G18), d-block (G3-G10), and d-block (G11-G12). Each of these blocks showed different range of k values indicating of different type of inner structure and inner electronic system. A brief review is shown below:

- s-block (H & He) showed k values between 1.35 to 2.
- s-block (G1, G2) had generally their k values between 0.5 to 1.
- p-block (G13-G18) had generally their k values between 0.5 to 1.
- d-block (G3-G10) had generally their k values less than 0.5.
- d-block (G11-G12) had generally their k values between 0.5 to 1.

The drop of k value below 0.5 for the d-block (G3-G10) indicated of much larger and more disorganized inner electronic systems. This group was the hardest to fit a simulating curve on their experimental data and their data sometimes showed a linear behavior. The rest of elements were similar and had their k values between 0.5 and 1.0 in general. The author does not understand much of the essence and sources of the differences.Table 1 presents the tabulated values of the characteristic exponent (k) for elements of periodic table with the corresponding average absolute error in eV. Most of the data available in the data bank was processed for this study.

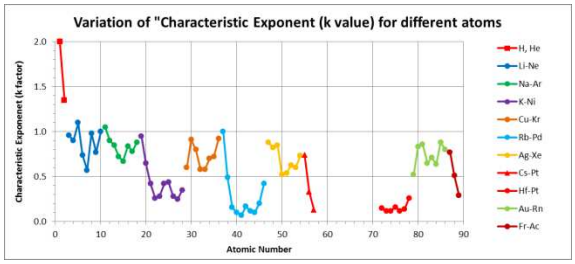

Figure 27: Variation of characteristic exponent k among elements of periodic table

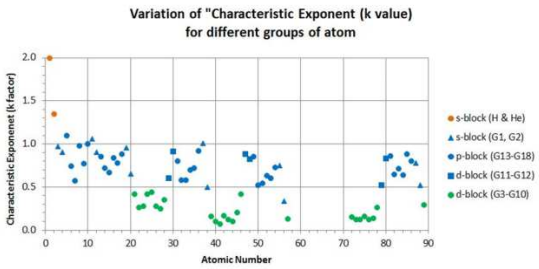

Figure 28: Variation of characteristic exponent k for different groups of atoms

Tabulated Characteristic Exponent (k)

A.N.	Name	k value	Avg. Error	A.N.	Name	k value	Avg. Error	A.N.	Name	k value	Avg. Error
1	H	2.00	0	26	Fe	0.28	1.06	51	Sb	0.54	0.27
2	He	1.35	0.23	27	Co	0.25	1.2	52	Te	0.63	0.45
3	Li	0.96	0.14	28	Ni	0.35	1.05	53	I	0.60	0.22
4	Be	0.90	0.2	29	Cu	0.60	0.56	54	Xe	0.73	0.3
5	B	1.10	0.21	30	Zn	0.91	0.37	55	Cs	0.74	0.19
6	C	0.74	0.38	31	Ga	0.80	0.29	56	Ba	0.33	0.42
7	N	0.57	0.26	32	Ge	0.58	0.53	57	La	0.13	0.21
8	O	0.98	0.4	33	As	0.58	0.45	72	Hf	0.15	0.25
9	F	0.77	0.38	34	Se	0.70	0.87	73	Ta	0.12	0.26
10	Ne	1.00	0.37	35	Br	0.72	0.35	74	W	0.12	0.24
11	Na	1.05	0.08	36	Kr	0.92	0.35	75	Re	0.16	0.22
12	Mg	0.90	0.18	37	Rb	0.92	0.09	76	Os	0.12	0.39
13	Al	0.85	0.05	38	Sr	0.49	0.27	77	Ir	0.14	0.69
14	Si	0.72	0.39	39	Y	0.16	0.39	78	Pt	0.26	0.5
15	P	0.67	0.4	40	Zr	0.10	0.2	79	Au	0.52	0.55
16	S	0.84	0.38	41	Nb	0.07	0.26	80	Hg	0.83	0.23
17	Cl	0.78	0.33	42	Mo	0.17	0.12	81	Tl	0.86	0.16
18	Ar	0.88	0.39	43	Tc	0.12	0.22	82	Pb	0.65	0.35
19	K	0.95	0.12	44	Ru	0.10	0.44	83	Bi	0.71	0.41
20	Ca	0.65	0.35	45	Rh	0.20	0.72	84	Po	0.64	0.56
21	Sc	0.42	0.59	46	Pd	0.42	0.66	85	At	0.88	0.44
22	Ti	0.26	0.8	47	Ag	0.88	0.27	86	Rn	0.80	0.22
23	V	0.28	0.78	48	Cd	0.82	0.29	87	Fr	0.77	0.18
24	Cr	0.42	0.63	49	In	0.85	0.22	88	Ra	0.51	0.41
25	Mn	0.44	0.62	50	Sn	0.52	0.31	89	Ac	0.29	0.52

Table 1: Tabulated characteristic exponent (k) for different elements of periodic table with the corresponding average absolute error in eV

Conclusion:

Most of the experimental energy levels of different elements available in NIST data bank were utilized for this study. The author did his best to separate the energy levels correctly and come up with a descent list of experimental data for the study and simulations. It seems that the methodology of predicting the excited energy levels for different elements suggested in this article works sufficiently well to simulate the behavior of atomic excited states. The mechanism of atomic excitation with the inner electrons in place and intact as suggested in this article is a new concept which may need further investigations. Also the introduction of "Characteristic Exponent k" together with the related ionization energies as a tool to mimic and simulate the excited energy levels of elements seemed effective and successful. Meanwhile, the characteristic exponent k showed potential to provide us with clues about the status of inner electrons of atoms as well as better understanding of their electronic structures. This article is considered a ground work for future developments.

Author Declaration:

1. Funding (information that explains whether and by whom the research was supported)
   There was no funding for this research work.
2. Conflicts of interest/Competing interests (include appropriate disclosures)
   There is no conflict of interest for this research work.
3. Availability of data and material (data transparency)
   All data and material were submitted with full transparency.
4. Code availability (software application or custom code)

There was no software or code prepared for this article.

5. Authors' contributions (include appropriate statements)
There is only one author who contributed all of the research work.

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