

**Title: An alternative equation for effective nuclear charge that
is applicable to all atoms**

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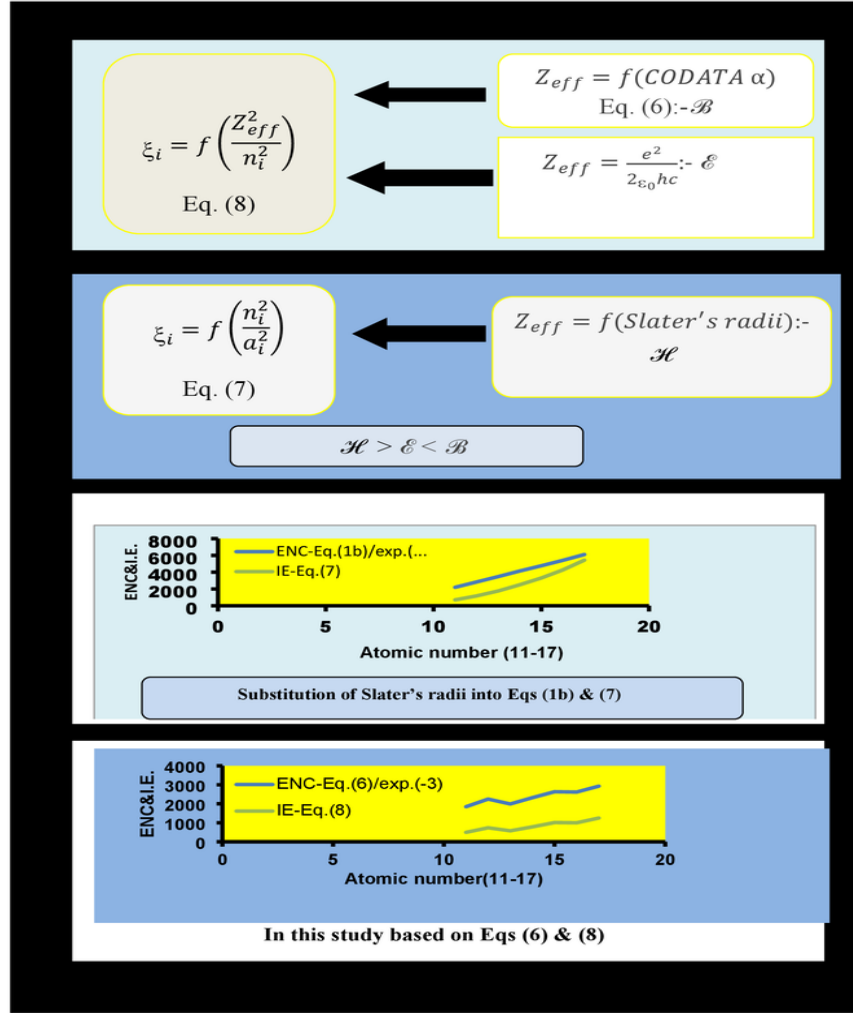
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Abstract

Although the advent of ionization energies predated Slater's rule, there was unawareness of the utilitarian value of the former for the computation of effective nuclear charge (ENC for short) until recently and in this research. The study aimed to derive another equation in which the average ionization energies of hydrogen and any other multi-electron atom are independent variables. The objective was to answer the question in the literature that states, "Are Slater's Rules the Best Approach for Calculating Effective Nuclear Charge for Undergraduates?" (Moore & Birnbaum, 2014) and compare the graphical portrayal of chemical periodicity between outcomes using data generated using Slater's rules for some elements and data generated in this research. By exploring theoretical and computational methods and the data in the literature, the study showed that ENC (1.34458-3.32446) for the first 30 elements computed using the 2021 CODATA fine structure constant (FSC, for short) was higher than those (1.34402-3.32309) without it; however, the equation containing the computed FSC using $e^2/2\epsilon_0hc$ and other equations gave the same value of ENC. The use of Slater's result (atomic radii) for the computation of ENC (1.29859-5.06996) and average ionization energy, IE (553.21-2108.13 kJ), gave higher values than other methods. All plots using Slater's values of ENC and IE versus atomic number (Z) did not show chemical periodicity (greater linearity), unlike the use of other values (less linearity or lower R^2). The new equation was derived, and with earlier equations, ENC can be accurately computed; they should therefore be part of the school curriculum at all levels without ceasing to teach Slater's rule, which is not the best approach. A future study should include 30 other elements of the periodic table.

Key words: Average ionization energy, effective nuclear charge, Slater's rule, Fine structure constant, Atomic radius, Chemical periodicity.

Graphical abstract



Introduction

Assumed inadequacies in Bohr's theory of the hydrogen atom—let alone multi-electron atoms—prompted the search for a more complex model. One such model treats the electron as a wave rather than a discrete particle. Schrödinger introduced this concept *via* his famous equation $E\psi = -\frac{\hbar^2}{2\mu}\nabla^2\psi + V(r)\psi$. In the Schrödinger equation, the parameter

E is the quantized energy, μ is the reduced mass, ∇^2 is the Laplacian operator representing the kinetic energy curvature in space, $V(r)$ is the potential energy based on Coulomb's law, and ψ is the wave function regarding the electron's quantum state. A parameter $|\psi|^2$ can be added to these: the probability density of finding the electron at a specific point in space. Past studies have shown that the average ionization energies of atoms can be used to calculate and map the probability density of locating an electron in any atom¹. A small magnitude of the probability function means that the average ionization-dependent radius of the atom is very large. The corollary is that the magnitude of the probability density should also be small if the effective nuclear charge is small, and *vice versa*. This is why the effective nuclear charge is a very important parameter in characterizing different elements.

Meanwhile, despite the advent of the average ionization energy of atoms of different elements, which predates the empirical equation developed by a US-born Slater², there has not been an appreciation of the usefulness of such all-important parameters that can define both chemical and physical characteristics of elements until recently, in articles authored by Udema^{3,4}. *Persons who either directly or indirectly contributed to the issue of ionization before Slater are German physicist Eugen Goldstein (1886), British Joseph John Thomson (1897), German American James Franck and German Gustav Hertz (1914), Canadian American Arthur Dempster (1918), and Soviet-era Nikolai Semyonov (1920s)*. What then is new? The fact is that average ionization energy is a function of the effective nuclear charge. There is an abundance of spectroscopic data in most rich, highly advanced scientific communities where the culture of science has been entrenched. As stated earlier, new versions of Bohr's equation and subsequent versions have explored average ionization energy on the web for the determination of effective nuclear charge of all elements, hydrogenic and nonhydrogenic alike. In answer to the question, this research aims to once again derive another equation in which the average ionization energies of hydrogen and any other element, be it either hydrogenic or nonhydrogenic multi-electronic, are independent variables for the computation of the effective nuclear charge of any atom. Ultimately, the objective is to answer another question in the literature that states, "Are Slater's Rules the Best Approach for Calculating Effective Nuclear Charge for Undergraduates?"⁵, and compare the graphical portrayal of chemical periodicity between outcomes using data generated using Slater's rules for some elements and data generated in this research

Theory

As this section would show, there has been concerted effort tailored towards the determination of effective nuclear charge. Using a semiempirical method that allows for spin-orbit interaction, a refined set of values for the effective nuclear charge and one-electron spin-orbit constants was obtained for transition metal ions, enabling the calculation of the spectrum of free ions. The

effective nuclear charge, a variable theoretical parameter that can be calculated based on spectroscopic data, was determined by comparing theoretically calculated ion absorption spectra with experimental ones⁶. However, the role of spin-orbit interaction and how these approaches—namely, the semiempirical method and absorption spectra—aid in determining the effective nuclear charge remains unclear.

Interestingly, some authors admit to the mathematical complexity involved in determining atomic structure, which could improve our understanding of elemental properties. For example, Slater integrals are considered two-dimensional radial integrals, and their integrand is constructed from normalized eigenfunctions of the Schrödinger equation⁷. Mere mention of Schrödinger equation eigenfunctions often conveys an air of mathematical complexity, as referenced by a no-nonsense American, Mills⁸. Although Slater integrals are used in many atomic and scattering computations, they pose a significant computational challenge in two-R-matrix propagation⁷. This concept is unfamiliar to most readers and is irrelevant to the method examined in this study. But why is the reference to spin-orbit? The simple answer is that it plays a role in determining the effective nuclear charge, and *vice versa*. For example, the effective nuclear charges of the main group elements from the second to the fifth row were developed using the one-electron part of the spin-orbit coupling Hamiltonian. These parameters are ideal for spin-orbit (SO) calculations of large molecular systems and offer a remarkably accurate approximation of the full SO Hamiltonian⁹. Besides, the effective nuclear charges (Z_{eff}), which are regarded as empirical parameters in an approximate spin-orbit Hamiltonian, were determined for the first-through third-row transition metal elements by exploring experimental results for the fine-structure splitting in atomic terms¹⁰. Honestly, only the original authors fully understand these methodologies and terms. Whatever the case, the average ionization energy of any atom is, from the perspective of Coulomb's law, directly proportional to the square of the latter (*i.e.* Z_{eff}) if Bohr's equation is substituted into Coulomb's equation. The average ionization energy, when determined experimentally, leads to the computation of the effective nuclear charge. However, this computation is somewhat indirect and can be considered semiempirical.

For non-hydrogenic atoms or ions, the commonly used definition of the effective nuclear charge (Z_{eff}) for a bound electron in an orbital (where n and l are the principal quantum number and angular momentum of the orbital, respectively) is defined according to the hydrogenic orbital energy formula (in atomic units): $E_{nl} = Z^2/2n^2$. Here, E_{nl} is the electron energy in the nl orbital. However, four alternative definitions of the effective nuclear charge (ENC or Z_{eff}) are presented that employ the orbital quantities $\langle r \rangle$, $\langle r^2 \rangle$, $\langle r^{-1} \rangle$ and $\langle r^{-2} \rangle$, and $\langle r^{-2} \rangle$. These can be expressed analytically using the hydrogen-like expectation values of $\langle r^k \rangle = \langle n, l | r^k | n, l \rangle$, as detailed by Li *et al.*¹¹. The five ENCs are defined by these five orbital quantities, which can be conveniently obtained using quantum-mechanical numerical calculations, such as the Multi-Configuration Dirac-Fock (MCDF) method employed in the study by Li *et al.*¹¹.

*As the foregoing review shows, the general observation in the literature is that many complex methods are explored despite the availability of spectroscopic data, such as the average ionization energy of elements up to the 5th energy level and beyond. According to Li *et al.*¹¹ and the existing literature, ENC (*i.e.* effective nuclear charge for short) is*

important for evaluating key atomic quantities, such as the cross sections of photon-atom and electron-atom collisions. ENC has recently been widely implemented in various atomic and plasma codes in the form of analytical formulae, which are useful simulation tools in fields such as nuclear fusion, astronomy, and light sources (see Li *et al.*¹¹ and the existing literature cited). While ENC is a significant concept for reflecting the net charge experienced by an electron in an atom or ion with multiple bound electrons, the idea that it enables such atoms or ions to be treated as hydrogenic atoms *via* an effective nuclear potential is inconsistent with the concept of hydrogenicity. The latter states that a hitherto multielectron atom or ion behaves similarly to a one-electron atom, such as hydrogen. All other atoms or ions must possess only one electron in the remaining orbital (or, more accurately, lowest energy level). All multielectron atoms have a decimal ENC for all energy levels except for the single-electron 1s orbital. This is why, similar to previous formulations or derivations, this study aims to derive a new equation for calculating the definite Z_{eff} of the first 30 elements of the periodic table as an illustration. It makes sense doing so because the magnitude of average ionization energy is a function of the atom's Z_{eff} . Strictly speaking, an atom is either hydrogenic or nonhydrogenic, such that the effective nuclear charge is equal to the difference between the atomic number and the screening constant. An effective nuclear charge alternative equation applicable to all atoms, which supports Bohr's theory, is derived in a very simple way for this assertion.

The concern for ENC, with a focus on undergraduates, has compelled some scholars to trace and analyze the primary and secondary historical sources, the progression, and the application of Slater's rules, as may have been observed in collegiate textbooks. Having reviewed a substantial number of collegiate inorganic textbooks, they realized limitations regarding Slater's rules that are worthy of discussion¹². This study has revealed the possibility of such shortcomings, and it would be appropriate to say no to the question, "Are Slater's Rules the Best Approach for Calculating Effective Nuclear Charge for Undergraduates?"⁵.

A well-known Bohr's equation is given as:

$$a_0 = \frac{n^2 h^2 \epsilon_0}{\pi m_e e^2 Z_{eff}} \quad (1a)$$

Setting aside the assumption that natural scientists understand the parameters in Eq. (1a), the terms are as follows: the principal quantum number; the Planck constant; the permittivity of free space; the mass of an electron; and the effective nuclear charge. These are represented by the letters and symbols, n , h , ϵ_0 , m_e , e , and Z_{eff} , respectively. The hydrogen atom is typically associated with equation (1a), which assumes $Z_{eff} = 1$ for the atom and any other higher hydrogenic atom with an atomic number greater than 1. Therefore, it is recognized that equation (1a) requires modification to account for the variety of atoms, resulting in the formula

$$a_i = \frac{n_i^2 h^2 \epsilon_0}{\pi m_e e^2 Z_{eff}} \quad (1b)$$

Where a_i and n_i are the Bohr radii of any atom and the principal quantum number, respectively. The phrase "Bohr radius of any atom" is a testament to the fact that Bohr is the author of the original equation upon which any modification arises. The challenge in the original Bohr's equation (Eq. (1b)) is that the effective nuclear charge (Z_{eff}) is not directly determinable. However, the 1930 Slater's rule attempted to do so. The 21st century equations^{3, 4} were, however, derived recently to solve such problem given experimental average ionization energies.

$$Z_{eff} = \frac{(8\xi_i)^{1/2} n_i h \epsilon_0}{m_e e^2} \quad (2)$$

$$Z_{eff} = \frac{n_i (2\xi_i)}{\alpha c (m_e)}^{1/2} \quad (3)$$

Where α and c are fine structure constant and the velocity of light in free space, respectively.

$$a_i = \frac{e^2 n_i}{8\pi\epsilon_0 (\xi_H \xi_i)^{1/2}} \quad (4)$$

Here, ξ_H and ξ_i represent the average ionization energy of a hydrogen atom and a different, non-hydrogenic element with a higher atomic number. Thus, Eqs (1b) and (2) are equivalent to each other, such that

$$\frac{n_i h^2 \epsilon_0}{\pi m_e e^2 Z_{eff}} = \frac{e^2}{8\pi\epsilon_0 (\xi_H \xi_i)^{1/2}} \quad (5)$$

$$\xi_H = 2.179872361 \text{ exp. } (-18)\text{J} = 0.5 \times a.u. \text{ of force} \times a_0. \text{ (CODATA, 2021)}$$

Solving for Z_{eff} gives the equation as follows:

$$Z_{eff} = \frac{8\epsilon_0^2 h^2 n_i (\xi_H \xi_i)^{1/2}}{m_e e^4} \quad (6)$$

$$(Z_{eff} = 0.999999999 (\approx 1) \text{ if } \xi_i = \xi_H.)$$

Earlier equations *i.e.* Eq. (2) and Eq. (3)^{3, 4} in alphabetical order can reproduce the same value of Z_{eff} .

Methods

The methods are theoretical and computational in nature; data in the literature, including spectroscopic data on the web, were explored for the evaluation of equations. Given known values of n_i , a_i , and ξ_H , the values of ξ_i made subject of the formula in Eq. (4) can be computed. The formula is as follows:

$$\xi_i = e^4 n_i^2 / 64 \pi^2 \epsilon_0 \xi_H a_i^2 \quad (7)$$

Another straightforward equation for average ionization is common in most textbooks and found to bear a negative sign, implying that it is the total energy (TE) in line with convention; by such convention, the potential energy (PE) is of the same sign as the total energy but twice in magnitude ($PE = -2TE$). “The foregoing claim is relevant at both the undergraduate and postdoctoral levels, barring unnecessary egotism!” However, the kinetic energy (KE) is of interest, and it is derived as follows: Substitute Eq. (1b) into Coulomb’s equation ($Z_{eff} e^2 / 8\pi\epsilon_0 a_i$) for KE to give the following equation.

$$\xi_i = \frac{m_e e^4 Z_{eff}^2}{8 n_i^2 h^2 \epsilon_0^2} \quad (8)$$

Waldron *et al.*¹³ suggested that freshmen and advanced students may use different methods to calculate screening percentage based on inner electrons, using a modified version of Slater’s method. However, this study challenges this approach, as a method that stands the test of time must produce the same results for the parameter of interest at all levels of academic achievement. As in previous studies^{3, 4}, the average ionization is strictly a function of the effective nuclear charge, reflecting the distance of the outer electron from the nucleus. The closer the electron is to the nucleus, the higher the average ionization energy and, consequently, the higher the effective nuclear charge.

“Scintillating crystals play a critical role in nuclear energy and radiation detection applications, such as nuclear batteries and radiation dose detectors. Both applications urgently require scintillation crystals with high radioluminescence efficiency”.¹⁴ Nuclear batteries, either beta-voltaic or alpha-voltaic, can generate more electricity when the radiation’s energy exceeds the average ionization energy (a function of Z_{eff}) of atoms in a semiconductor or gas medium, creating charge carriers that accumulate. If the average ionization energy of the converter material is much higher than the particle’s energy, fewer electron-hole pairs form, lowering the battery’s net electrical output and efficiency.

The effective nuclear charge (ENC) values were computed for the first 30 elements of the periodic table. The CODATA value of the fine structure constant and the average ionization energy (I.E.) of each element were substituted into Eq. (3) given values shown in Table 1. The reproducibility of I.E. was verified by substituting two versions of Bohr’s radius for hydrogen arising from the substitution of rest mass and reduced mass into the Bohr’s equation for hydrogen radius (Eq. (1b)) into Coulomb’s equation. As expected, the verification yielded slightly different values, A and B (Table 1) that should not be ignored.

Table 1: Ground state outer most energy level effective nuclear charge determination based on Eq. (3) for the first 30 elements of the Periodic Table

Elements	Electronic structure	Effective nuclear charge	Average ionization energy/kJ/mol	
			A	B

H	1s ¹	-	-	-
He	1s ²	1.344576148	2372.345863	2373.301002
Li	[He]2s ¹	1.259261043	520.2100569	520.4195005
Be	[He]2s ²	1.655888835	899.5173898	899.875477
B	[Be]2p ¹	1.561913586	800.3154722	800.6376901
C	[Be]2p ²	1.819881344	1086.521005	1086.958453
N	[Be]2p ³	2.067526387	1402.32711	1402.891706
O	[Be]2p ⁴	2.001297949	1313.925401	1315.636913
F	[Be]2p ⁵	2.263676961	1681.032498	1681.709305
Ne	[Be]2p ⁶	2.518461567	2080.740226	2081.57796
Na	[Ne]3s ¹	1.844060283	495.8095852	496.0092048
Mg	[Ne]3s ²	2.249374383	737.7142617	738.0112755
Al	[Ne]3s ² 3p ¹	1.990205158	577.5152052	577.7436784
Si	[Ne]3s ² 3p ²	2.322582859	786.5152052	786.8318668
P	[Ne]3s ² 3p ³	2.634324013	1011.819561	1012.226933
S	[Ne]3s ² 3p ⁴	2.618393878	999.6193253	1000.226933
Cl	[Ne]3s ² 3p ⁵	2.929444139	1251.224189	1251.727949
Ar	[Ne]3s ² 3p ⁶	3.229455809	1520.629397	1521.241623
K	[Ar]4s ¹	2.259768374	418.8080965	418.97671391
Ca	[Ar]4s ²	2.681717177	589.8479651	590.0488084
Sc	[Ar]3d ¹ 4s ²	2.778412642	633.1122395	633.3671391
Ti	[Ar]3d ² 4s ²	2.834244973	658.8127364	659.0779833
V	[Ar]3d ³ 4s ²	2.817200293	650.9125817	651.1746479
Cr	[Ar]3d ⁴ 4s ²	2.821525139	652.9125963	653.1754677
Mn	[Ar]3d ⁵ 4s ²	2.957406278	717.3138189	717.6026191
Fe	[Ar]3d ⁶ 4s ²	3.0491621	762.5147389	762.8217377
Co	[Ar]3d ⁷ 4s ²	3.044960364	760.4147007	760.720854
Ni	[Ar]3d ⁸ 4s ²	2.997945927	737.1142501	737.4110223
Cu	[Ar]3d ⁹ 4s ²	3.014979841	745.5144094	745.8145636
Zn	[Ar]3d ¹⁰ 4s ²	3.324455603	906.4166273	906.7815629

A represents average ionization energy of hydrogen atom computed by fitting Coulomb's equation to the 2021 CODATA value of Bohr's radius ($a_0 = 5.29177210903 \exp.(-11)$ m, similar to $5.292523859 \exp.(-11)$ m computed based on the substitution of reduced mass ($9.104425278 \exp.(-31)$ kg) of the electron into original Bohr's equation ($n_i^2 h^2 \epsilon_0 / \pi m_e e^2 Z_{eff}$) for a_0 ; $Z_{eff} = 1$ if hydrogen atom is referred to. B represents average ionization energy of hydrogen atom computed by fitting Coulomb's equation to the Bohr's radius ($5.289643031 \exp.(-31)$ kg) computed by fitting Bohr's equation to the rest mass (2021, CODATA value is equal to $9.1093837015 \exp.(-31)$ kg) of the electron. Equation (3) was fitted to 2021, CODATA value of fine structure constant given as $7.2973525693 \exp.(-3)$.

Meanwhile, Table 2 showcases the same parameters computed based on Eq. (6) that was derived in this study. The equation contains the symbols for I.E. for hydrogen and any other atom. Substituting similar but different values of I.E. for hydrogen and I.E. for any other element gave slightly different values of ENC; substitution of these values of the latter into Eq. (8) expectedly gave different values of I.E. for each element. The obvious

reason is the use of two different values of I.E. for hydrogen; an exact experimental value of I.E. can obviate this challenge.

Table 2: Ground state outer most energy level effective nuclear charge determination based on Eq. (6) for the first 30 elements of the Periodic Table

Elements	Electronic structure	Effective nuclear charge		Average ionization energy/kJ/mol	
		A	B	A	B
H	$1s^1$	0.999597662	0.999999998	1312.221651	1312.74982
He	$1s^2$	1.344022183	1.344292639	2370.391455	2372.299998
Li	$[\text{He}]2s^1$	1.258742227	1.258995523	519.7814928	520.1999996
Be	$[\text{He}]2s^2$	1.258742227	1.258995523	898.7763404	899.49999941
B	$[\text{Be}]2p^1$	1.561270078	1.561584251	799.65619851	800.2999997
C	$[\text{Be}]2p^2$	1.819141549	1.819507614	1086.103121	1086.500
N	$[\text{Be}]2p^3$	2.066674567	2.067090443	1401.171831	1402.300
O	$[\text{Be}]2p^4$	2.000473415	2.000875969	1312.84295	1313.900
F	$[\text{Be}]2p^5$	2.262744327	2.263199657	1679.647613	1680.999999
Ne	$[\text{Be}]2p^6$	2.517423961	2.517930541	2079.02605	2080.699999
Na	$[\text{Ne}]3s^1$	1.843300531	1.843671457	495.4011224	495.7999997
Mg	$[\text{Ne}]3s^2$	2.24844764	2.248900095	737.1065101	737.699997
Al	$[\text{Ne}]3s^23p^1$	1.989385193	1.989785516	577.0353934	577.4999999
Si	$[\text{Ne}]3s^23p^2$	2.321625955	2.322093135	785.8672505	786.4999999
P	$[\text{Ne}]3s^23p^3$	2.633238671	2.633768557	1010.985993	1011.800
S	$[\text{Ne}]3s^23p^4$	2.6173151	2.61784178	998.7958087	999.5999993
Cl	$[\text{Ne}]3s^23p^5$	2.928237208	2.928826456	1250.041189	1251.200
Ar	$[\text{Ne}]3s^23p^6$	3.228125274	3.228774868	1519.376657	1520.599999
K	$[\text{Ar}]4s^1$	2.258837349	2.259291894	418.4630699	418.7999999
Ca	$[\text{Ar}]4s^2$	2.68061231	2.681151728	589.3254982	589.7999997
Sc	$[\text{Ar}]3d^14s^2$	2.777267937	2.777826805	632.5906628	633.0999998
Ti	$[\text{Ar}]3d^24s^2$	2.833077264	2.833647363	658.2699868	658.7999998
V	$[\text{Ar}]3d^34s^2$	2.816039611	2.816606281	650.3763424	650.8999998
Cr	$[\text{Ar}]3d^44s^2$	2.820302671	2.820930211	652.2953106	652.900
Mn	$[\text{Ar}]3d^54s^2$	2.956187927	2.956782799	716.7229228	717.2999998
Fe	$[\text{Ar}]3d^64s^2$	3.047505851	3.048519179	761.8865588	762.4999997
Co	$[\text{Ar}]3d^74s^2$	3.047905851	3.044318324	759.7882482	760.3999994
Ni	$[\text{Ar}]3d^84s^2$	2.996710773	2.9973138	736.5069934	737.0999999
Cu	$[\text{Ar}]3d^94s^2$	3.013737676	3.014344129	744.9002355	745.4999997
Zn	$[\text{Ar}]3d^{10}4s^2$	3.323085933	3.323754635	905.6707893	906.3999997

A & B are as defined under Table 1. Equation (6) was explored.

The 1930 data for atomic radii of the first 30 elements, excluding 4 elements, were explored for the computation of average ionization energy using Eq. (7). The values of the computed average ionization energies (Table 3) were approximately 1.3 to 5-fold higher than values recorded in Tables 1 and 2. This clearly showed that the radii of atoms based on Slater's rule are much less than those expected from the use of Eqs. (4), given spectroscopic data on I.E. available on the web.

Table 3: Average ionization energies for the first 30 elements less four of the Periodic Table based on Eq. (4) and the use of Slater's data (Slater, 1930)

Elements	Electronic structure	Radii/Å Based on Slater's rule	Average ionization energy/kJ/mol	
			A	B
H	1s ¹	-	-	-
He	1s ²	-	-	-
Li	[He]2s ¹	1.63	553.215383	551.621394
Be	[He]2s ²	1.09	1237.133196	1236.6354
B	[Be]2p ¹	0.82	2185.95769	2185.078198
C	[Be]2p ²	0.65	3478.906393	3477.506375
N	[Be]2p ³	0.55	4858.968433	4857.013489
O	[Be]2p ⁴	0.47	6653.861254	6651.1841571
F	[Be]2p ⁵	0.41	8743.83074815	8740.316986
Ne	[Be]2p ⁶	-	-	-
Na	[Ne]3s ¹	2.17	702.3159102	702.0333423
Mg	[Ne]3s ²	1.68	1171.74581	1171.274378
Al	[Ne]3s ² 3p ¹	1.37	1762.020028	1761.310092
Si	[Ne]3s ² 3p ²	1.15	2500.784439	2499.663369
P	[Ne]3s ² 3p ³	1.00	3307.13539	3305.804806
S	[Ne]3s ² 3p ⁴	0.88	4270.577725	4268.859511
Cl	[Ne]3s ² 3p ⁵	0.78	5436.453095	5434.265808
Ar	[Ne]3s ² 3p ⁶	-	-	-
K	[Ar]4s ¹	3.32	533.4003306	533.1857229
Ca	[Ar]4s ²	2.56	897.11789	896.7569459
Sc	[Ar]3d ¹ 4s ²	2.43	995.6733904	995.2727939
Ti	[Ar]3d ² 4s ²	2.32	1092.329036	1091.889551
V	[Ar]3d ³ 4s ²	2.22	1192.953454	1192.473484
Cr	[Ar]3d ⁴ 4s ²	2.12	1308.150543	1307.624225
Mn	[Ar]3d ⁵ 4s ²	2.02	1440.876336	1440.296617
Fe	[Ar]3d ⁶ 4s ²	1.95	1546.180618	1545.558532
Co	[Ar]3d ⁷ 4s ²	1.87	1681.303956	1680.627505
Ni	[Ar]3d ⁸ 4s ²	1.80	1814.8357	1814.105524
Cu	[Ar]3d ⁹ 4s ²	1.73	1964.433093	1963.642728

Zn	[Ar]3d¹⁰4s²	1.67	2108.125692	2107.874949
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A & B are as defined under Table 1. The solution of ξ_i in Eq. (4) is for the sake of quick reference given as:

$$\xi_i = e^4 n_i^2 / 64 \pi^2 \epsilon_0 \xi_i a_i^2$$

As a fallout from the observation in Table 3 (larger I.E.), the corresponding computed effective nuclear charges (Table 4) based on Coulomb's equation for kinetic energy were expectedly higher by between 1.129 and 2.28-fold than those recorded in Tables 1 and 2.

Table 4: Effective nuclear charge computed using the radii computed according to Slater's rule.

Elements	Electronic structure	Effective nuclear charge	
		A	B
H	1s ¹	-	-
He	1s ²	-	-
Li	[He]2s ¹	1.298594377	1.294852536
Be	[He]2s ²	1.941934712	1.9411534
B	[Be]2p ¹	2.58135224	2.580313672
C	[Be]2p ²	3.256475135	3.25516464
N	[Be]2p ³	3.848561535	3.847013115
O	[Be]2p ⁴	4.503635839	4.501823859
F	[Be]2p ⁵	5.162704489	5.160629824
Ne	[Be]2p ⁶	-	-
Na	[Ne]3s ¹	2.197288187	2.196390851
Mg	[Ne]3s ²	2.834877916	2.833737339
Al	[Ne]3s ² 3p ¹	3.476346642	3.474945987
Si	[Ne]3s ² 3p ²	4.141386869	4.139720634
P	[Ne]3s ² 3p ³	4.762594899	4.760637435
S	[Ne]3s ² 3p ⁴	5.412714955	5.409878516
Cl	[Ne]3s ² 3p ⁵	6.106634344	6.104177417
Ar	[Ne]3s ² 3p ⁶	-	-
K	[Ar]4s ¹	2.550271774	2.549225574
Ca	[Ar]4s ²	3.307357791	3.306027152
Sc	[Ar]3d ¹ 4s ²	3.484294628	3.482892766
Ti	[Ar]3d ² 4s ²	3.649498222	3.648029894
V	[Ar]3d ³ 4s ²	4.1821776603	4.180493956
Cr	[Ar]3d ⁴ 4s ²	3.993790269	3.992183417
Mn	[Ar]3d ⁵ 4s ²	4.19150266	4.189816264
Fe	[Ar]3d ⁶ 4s ²	4.341966703	4.340219767
Co	[Ar]3d ⁷ 4s ²	4.527719757	4.526449154
Ni	[Ar]3d ⁸ 4s ²	4.704370477	4.702477733
Cu	[Ar]3d ⁹ 4s ²	4.894124755	4.892290726
Zn	[Ar]3d ¹⁰ 4s ²	5.069961246	5.06935822

A & B are as defined under Table 1. The equation of Z_{eff} derived from Coulomb's equation for average ionization energy is for the sake of quick reference given as follows: $Z_{eff} = e^2 / 8\pi\epsilon_0 \xi_i a_i$; substitution of Slater's radii (a_i) and ξ_i (Table 3) into the latter gives after calculation the values of effective nuclear charge.

The all-important question now is that of the periodicity of the elements; this shows how any periodic property influenced by the nuclear medium varies across the periodic table. When looking at the periodic table, one will always come across metals, metalloids, and non-metals. This classification of elements also shows different ENC values that demonstrate nonlinearity across the periodic table (Figure 1). The same scenario applies to a plot of I.E. versus the atomic numbers (11–17) of the elements. The coefficients of determination (0.874 and 0.870) express imperfect linearity.

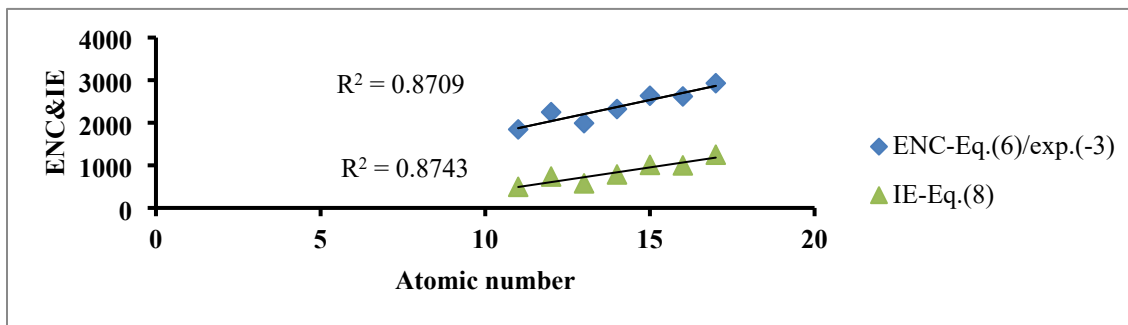


Figure 1: A plot of effective nuclear charge, ENC (Z_{eff}), and average ionization energy, I.E. (ξ_I) versus atomic number (Z)-This study. $\diamond$: ENC was computed based on the use of spectroscopic data (I.E.) available on the internet to which was fitted Eq. (6). Δ : The I.E. values were reproduced by computation after substituting the ENC in this study into Eq. (8).

A close observation of Figure 2 revealed coefficients of determination (0.999 and 0.979) that are greater than those observed in Figure 1. The greater linearity indicates a clear absence of chemical periodicity. The implication is that the radii of elements determined for about 26 elements using Slater's rule and reported in the literature are inappropriate. A similar view had been held regarding the appropriateness of Slater's rules for calculating Z_{eff} for undergraduates⁵. This study does not promote a double standard in which top scientists have exclusive equations and methodologies that differ from those used by undergraduates. If the equations and methodologies are not suitable for teachers, they are not suitable for students. While the periodic behavior of Z_{eff} calculated using Slater's rules roughly matches the periodicity of gas-phase ionization energies (IEs), the IEs calculated using the equation $IE = (Z_{eff}/n^*)^2$ fit poorly for all ns- and np-subshell elements⁵. Despite an alternative method proposed by the same authors⁵, no better result can be expected from an equation relating Z_{eff} to the underlying effect of average ionization energy. This study showcases this fact.

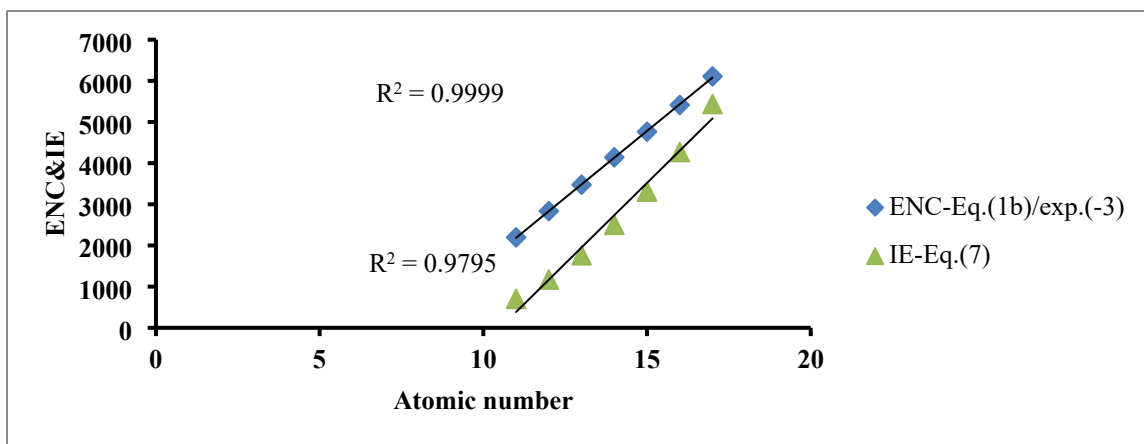


Figure 2: A plot of effective nuclear charge, ENC (Z_{eff}), and average ionization energy, I.E. (ξ_I) versus atomic number (Z)-Slater' parameter. $\diamond$: ENC was computed based on the use of Slater's radii to which was fitted Eq. (1b). Δ : The I.E. values were computed by substituting the Slater's radii into Eq. (7).

It is now imperative to inform core physicists and chemists that novelty is not necessarily rooted in mathematical complexity. Much of this complexity arose after the work of Dirac, Schrödinger, and others. There is nothing wrong with teaching Slater's rule at the undergraduate level, in the same way that the two theories that preceded the chemiosmotic theory are taught. The new equations derived so far should therefore be made an integral part of the curriculum at all levels. The equations (Eqs. 2 & 3) that are already in the literature and Eq. (6) can be explored for the computation of effective nuclear charge values, which can display chemical periodicity when plotted versus atomic number. The applications of effective nuclear charge require correctly computed values based on time-tested average ionization using the new equations in the past and in this study. The advocates of complex mathematization of the description of electronic structure are reminded that Bohr's original theory and equation are only applicable to the outermost energy level, or better yet, the outermost shell. As of this moment, there is no high-tech device that can knock out the penultimate electron from its orbital.

Conclusion

The equation for the computation of effective nuclear charge was derived, adding to earlier versions. The use of Slater's result (atomic radii) for the computation of ENC (1.29859-5.06996) and average ionization energy, IE (553.21-2108.13 kJ), gave higher values than other methods. All plots using Slater's values of ENC and IE versus atomic number (Z) did not show chemical periodicity (greater linearity), unlike the use of other values (less linearity or lower R^2). The new equation was derived, and with earlier equations, ENC can be accurately computed; they should therefore be part of the school curriculum at all levels without ceasing to teach Slater's rule, which is not the best approach. A future study should include 30 other elements of the periodic table. Inconsistent periodic properties due to the CODATA fine structure constant and reduced mass do not totally repudiate chemical periodicity

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Conflict of Interests

The author declares no conflict of interest

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Authors Contributions

The sole author designed, analyzed, interpreted and prepared the manuscript.

Availability of Data and Materials

Spectroscopic data (average ionization energy) can be found on the web; radii of atoms are available in the literature (Slater, 1930).

Disclaimer (Artificial Intelligence)

The author(s) hereby declare(s) that no generative AI technologies, such as Large Language Models (ChatGPT, COPILOT, *etc.*) and text-to-image generators have been used during the writing or editing of this manuscript. Note that Quillbot only edits the manuscript (spell-checking, punctuation, *etc.*) before it, while ChatGPT and COPILOT create a brand new manuscript from scratch for the author(s).

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