# New Equations for Calculating Principal and Fine-Structure Atomic Spectra for Single and Multi-Electron Atoms

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A set of equations are presented for calculating atomic principal spectral lines and fine-structure energy splits for single and multi-electron atoms. Calculated results are presented and compared to the National Institute of Science and Technology database demonstrating very good accuracy. The equations do not require fitted parameters. The only experimental parameter required is the Ionization energy for the electron of interest. The equations have comparable accuracy and broader applicability than the single electron Dirac equation. Three Appendices discuss the origin of the new equations and present calculated results. New insights into the special relativistic nature of the Dirac equation and its relationship to the new equations are presented. NETL-PUB-21635

Key words: Atomic Spectra; Multi-Electron Atom; Principal Spectral Line; Atomic Fine-Structure; Special Relativity; Dirac Equation

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# 1. Introduction

The initial purpose of this paper was to validate previously (unpublished) discovered relationships to a definitive case where excellent and credible data exist to demonstrate that the physical relationships have a more general validity. The previous work suggested a relationship between the de Broglie wave and Coulomb potential which is further developed in this paper along with additional results including a new quantum relation and a new application of special relativity. These combined new developments result in a tractable methodology for calculation of principal spectra and fine-structure energy splits for any atomic electron, single or multi, in a theoretically justified, accurate and reliable way. The results of this paper far exceeded the original expectations.

The reported accuracies are determined by comparison of calculation to data, when it exists, reported in the National Institute of Standards and Technology (NIST) atomic spectra database [1]. The development of the equations follow from a specific set of ideas that draw on well-established and accepted physics constructs but assembled in an unconventional way. It is felt the successful outcome of the work should be published given that it is a theoretical development that might be of deeper interest and on a practical level can be used to calculate electron energy states with good accuracy requiring no fitted parameters. Given the simplicity, reliability and accuracy, it could also be useful for first order calculation of principal and fine-structure spectra for cases where data does not exist which could be of interest in spectroscopic and/or astronomical applications.

From a theoretical perspective, some intriguing discoveries and principles emerged that lead directly to the equations presented. The most important of these relates to the nature of the Dirac solution for hydrogen. It can be definitively shown that one characteristic of the Dirac solution is a special relativistic mass/wave correction or defect. This would be at least interesting, except that it leads to extension of the new equations for principal spectra developed in this paper to atomic fine-structure, with applicability to the fine-structure of multi-electron atoms.

Current methods for calculating spectra are described in papers published by the National Institute of Standards and Technology (NIST) [2,3] The methods are largely based on an empirical Rydberg-Ritz equation fitted to an expanded quantum defect with a host of individual corrections applied in bookkeeping fashion. They can be relatively complicated making them cumbersome and in most cases impractical to use [3,4]. The first equation presented in this paper for the principal spectral lines results in a non-fitted theoretically definitive Rydberg-Ritz type equation, eliminating the quantum defect. The new equation is consistently accurate compared to the NIST spectral database [1], single or multi-electron. For single electron principal lines and associated fine-structure the results are comparable in accuracy to the Dirac solution for single electrons, but, importantly, the equations prove accurate for multi-electron cases where the Dirac equation cannot be used in any direct way.

It is hoped these results provide increased opportunity for a simple, accurate and tractable method when used alone or when coupled with Quantum Electrodynamic (QED) corrections, depending on application.

# 2. General Calculation of Single or Multi-Electron Principal Spectral Lines

A new equation consistent with the Rydberg-Ritz form is presented for the moment without justification.

$$\boxed{E_{spectra} = I_e - \frac{I_e R_\infty}{\left(\sqrt{R_\infty} + \left(\frac{x}{a}\right)\sqrt{I_e}\right)^2}} \qquad (1)$$

Unlike the Rydberg-Ritz equation, Eq. 1 does not require or utilize any fitted parameters such as a quantum defect or $Z_{eff}$. It is applicable to any electron state for any single or multi-electron atom. It can be used to calculate the principal quantum number states or principal spectral lines and can be used in conjunction with relativistic and/or QED corrections which require a principal quantum number solution as a starting point. The derivation of Eq. 1 will be presented in Appendix A. The derivation is somewhat lengthy but richer in content than Eq. 1's simplicity suggests. A small sample of principal spectral line results for Eq. 1 are presented and compared to single-electron NIST experimental and Dirac solution results in Tables 1 and 2 and compared to NIST multi-electron experimental results in Table 3 of Section 3. More extensive results are presented in Appendix B.

The following parameters are used in Eq. (1),

$x$ = the principal energy transition – 1st transition $x$ = 1; 2nd transition $x$ = 2; and so on

$a$ = the electron number. For the outer electron $a$ = 1; $a$ ranges from Z to 1

$I_e$ = the Ionization energy for the electron of interest (eV). The Ionization energy is the principal ground state in this approach and is labeled $I_e$ for that reason.

$R_\infty$= the Rydberg constant or 'reduced' Rydberg constant (eV)

Equation (1) has the form of the Rydberg-Ritz combination principle which is currently used to fit spectral results, by interpolation or extrapolation. The current and standard form of the Rydberg-Ritz equation is typically written [5],

$$T = A - \frac{(Z - \delta_o)^2 R_\infty}{(m + a)^2}$$

where A is empirically but not theoretically justified to be the Ionization Potential and $(Z - \delta_o)$ is essentially a $Z_{eff}$ or more commonly referred to as the quantum defect and can be expanded to higher powers. The Rydberg-Ritz equation is currently used to fit some spectral data in the NIST database and/or other calculations where measured values do not exist [2,3,4].

The accuracy of Eq. 1 without correction is quite good and the calculation obviously very simple. In fact, for hydrogen and helium, as shown in Tables 1 through 3 of the next section, the accuracy compared to NIST spectral lines is comparable to the Dirac equation for the single electron case and is very accurate compared to the NIST database for the helium multi-electron case where the Dirac equation cannot be used for comparison. Another immediate observation is the convergence with zero deviation on the NIST line as the transition number increases.

Importantly, Eq. (1) can be applied to multi-electron atoms. The accuracy of Equation (1) is very good for any single or multi-electron atom where data was available for comparison.

## 3. Example: Principal Spectral Lines for H I, He II, and Multi-Electron He I Compared to the Dirac Equation and NIST

Results calculated using Equation (1) are presented in Tables 1., 2. and 3. for Hydrogen, and both Helium electrons. The single electron cases for H I and He II are compared to both NIST and the Dirac equation. The multi-electron case for Helium I is compared to NIST but not the Dirac equation.

In the case of H I and He II, Transitions 100 and 1000 are included for both Eq (1) and the Dirac equation to demonstrate that they converge and do not diverge as transitions increase. The principal spectral line for He I is the midpoint energy of the triplet and singlet states. This convention is used throughout for multiple electron atoms. There is not a direct correspondence between standard nomenclature and Equation (1). The principal line split for a two-electron atom was not explored, but if explored in the context of this paper, would most likely be characterized as an energy level split resulting from a special relativistic relationship for the two electrons in the same period. This type of relationship is explored in subsequent sections of this paper and leads to the fine-structure energy splits for single and multi-electron atoms.

## Table 1: Principal Spectral Lines - H (eV)

| **Principal Atomic Transition Number (x)** | **1** | **2** | **3** | **7** | **100** | **1000** |
|---|---|---|---|---|---|---|
| **Eq. 1 $I_e R_\infty$** | 10.19791879 | 12.08695976 | 12.74819214 | 13.38585972 | 13.59710073 | 13.59842091 |
| **Δ** | 8.9E-04 | 5.4E-04 | 3.4E-04 | 1.0E-04 | - | - |
| **NIST** | 10.19881044 | 12.08749486 | 12.74853289 | 13.38596004 | - | - |
| **Dirac $I_e m_e$** | 10.19695475 | 12.08667075 | 12.74806951 | 13.38584426 | 13.59710073 | 13.59842091 |
| **Δ** | 1.9E-03 | 8.2E-04 | 4.6E-04 | 1.2E-04 | - | - |

**$I_e =$ 13.598434486 (eV)**
**$m_e =$ 9.10938291E–31 (kg)**
**$R_\infty =$ 13.60569253 (eV)**
**Δ = the Absolute Difference between the calculated result and the NIST [1] value.**
**The Principal Atomic Transition Number is x. The Principal Quantum Number is n = x+1**

## Table 2: Principal Spectral Lines – He II (eV)

| **Principal Atomic Transition Number (x)** | **1** | **2** | **3** | **7** | **100** | **1000** |
|---|---|---|---|---|---|---|
| **Eq. 1 $I_e R_\infty$** | 40.81269816 | 48.37097595 | 51.01642011 | 53.56741902 | 54.41242999 | 54.41771072 |
| **Δ** | 3.9E-04 | 3.4E-04 | 2.5E-04 | 8.7E-05 | - | - |
| **NIST** | 40.81308859 | 48.37131431 | 51.01666808 | 53.56750616 | - | - |
| **Dirac $I_e R_\infty$** | 40.81117123 | 48.37047597 | 51.01620051 | 53.56738873 | 54.41242998 | 54.41771072 |
| **Δ** | 1.9E-03 | 8.4E-04 | 4.7E-04 | 1.2E-04 | - | - |

**$I_e =$ 54.41776503 (eV)**
**$m_e = 9.10938291E-31$ (kg)**
**$R_\infty =$ 13.60569253 (eV)**

## Table 3: Principal Spectral Lines – He I (eV)

| **Principal Atomic Transition Number (x)** | **1** | **2** | **3** | **7** | **8** | **9** |
|---|---|---|---|---|---|---|
| **Eq. 1 $I_e R_\infty$** | 20.11348748 | 22.78025732 | 23.61670827 | 24.36050516 | 24.40943304 | 24.44408537 |
| **Δ** | 1.0E-01 | 3.9E-02 | 1.7E-02 | 2.1E-03 | 1.5E-03 | 1.1E-03 |
| **NIST** | 20.2176948 | 22.8193920 | 23.6337648 | 24.3626422 | 24.4109319 | 24.4451768 |

**$I_e =$ 24.587388804 (eV)**
**$R_\infty =$ 13.60569253 (eV)**

# 4. The Principal Transition Energy and the Dirac Equation in the context of a Relativistic Mass Defect, Photon Wavelength Defect or De Broglie Wavelength Defect

The Dirac solution for the energy of an electron state is written as

$$E_e = m_e c^2 \left[ 1 - \left( 1 + \left[ \frac{Z\alpha}{n - j - ½ + \sqrt{(j + ½)^2 - Z^2\alpha^2}} \right]^2 \right)^{-½} \right]$$

The Dirac solution can be used a priori for calculating the principal states and fine-structure energy splits for single-electron but not multi-electron atoms given its reliance on the atomic number Z. The Dirac solution is very accurate for single-electron atoms. The Dirac equation is relativistic, unlike the Schrodinger equation, given that its derivation starts with the relativistic energy-momentum equation, and it is first order in both time and space coordinates, treating time and space on the same basis, a requirement of special relativity.

A key result of this paper is an even stronger more direct connection between the Dirac solution and special relativity which leads to new and intriguing results. It can be shown that the Dirac solution calculates the relativistic mass change of the transition energy due to the long held special relativistic requirement that any change in energy is equivalent to a change in mass. The most interesting finding is that the identical mass change can also be calculated based on the linear kinetic velocity using the state to state transition energy. This is demonstrated in Tables 4. And 5 for hydrogen and helium. As discussed in Appendix A, this is supported by calculations showing that a mass change or binding energy mass defect could well be the source of the ground state or ionization energy of hydrogen (and all other atoms by extension although the nuclear binding energy or mass defect of multi-nucleon atoms masks the small effect of the ionization energy), and suggests that succeeding transitions could/should also result from a change in mass or binding energy. This will be explored further.

The results of Tables 4 and 5 are calculated as follows. A term identified as Dirac γ in the tables is calculated according to

$$\text{Dirac}\,\gamma = \left( 1 + \left[ \frac{Z\alpha}{n - j - ½ + \sqrt{(j + ½)^2 - Z^2\alpha^2}} \right]^2 \right)^{½}$$

which is by inspection the principle part of the Dirac equation.

The term γ is the traditional special relativistic velocity dependent term with velocity calculated from the transition energy as a linear kinetic velocity. Angular velocity was explored but clearly did not give reasonable results. There does not appear to be any angular character in this methodology.

$$\gamma = \frac{1}{\sqrt{1-\left(\frac{v}{c}\right)^2}}$$

Which is identical to

$$\text{SR}\,\gamma = \frac{1}{\sqrt{1-\frac{2E_e}{m_e c^2}}}$$

where $E_e$ is the transition energy between states.

The values for Dirac γ and SR γ are compared for H I and He II in Tables 4 and 5.

## Table 4: Dirac γ compared to SR γ – H I (eV)

| **Principal Atomic Transition Number (x)** | **1** | **2** | **3** | **4** | **9** | **19** |
|---|---|---|---|---|---|---|
| **NIST $E_e$** | 3.399624046 | 1.510939626 | 0.849901596 | 0.543936136 | 0.135983505 | 0.033995746 |
| **Dirac $\gamma$** | 1.000006657 | 1.000002959 | 1.000001664 | 1.000001065 | 1.000000266 | 1.000000067 |
| **SR $\gamma$** | 1.000006653 | 1.000002957 | 1.000001663 | 1.000001064 | 1.000000266 | 1.000000067 |

**$I_e = 13.598434486$**
**$m_e = 9.10938291E-31$**
**NIST – the NIST [1} values for the Principal Spectral Line subtracted from the Ionization Energy.**
**The Principal Atomic Transition Number is x. The Principal Quantum Number is n = x+1**

## Table 5: Dirac γ compared to SR γ – He II (eV)

| **Principal Atomic Transition Number (x)** | **1** | **2** | **3** | **4** | **9** | **19** |
|---|---|---|---|---|---|---|
| **NIST $E_e$** | 13.60467644 | 6.04645072 | 3.40109695 | 2.17668761 | 0.54416338 | 0.1360383 |
| **Dirac $\gamma$** | 1.000026628 | 1.000011835 | 1.000006657 | 1.000004260 | 1.000001065 | 1.000000266 |
| **SR $\gamma$** | 1.000026625 | 1.000011833 | 1.000006656 | 1.000004260 | 1.000001065 | 1.000000266 |

**$I_e = 54.41776503$**
**$m_e = 9.10938291E-31$**
**NIST – Is the NIST [1} values for the Principal Spectral Line subtracted from the Ionization Energy.**
**The Principal Atomic Transition Number is x. The Principal Quantum Number is n = x+1**

Following this methodology, the Dirac solution for the transition energies can be written as,

$$E_e = m_e c^2 \left(1 - \frac{1}{\text{Dirac}\,\gamma}\right) = m_e c^2 \left(1 - \frac{1}{\gamma}\right)$$

or

$$E_e = m_e c^2 - \frac{m_e c^2}{\gamma} \tag{2}$$

which is identical to the Dirac equation and directly states that the transition energy is due to a change in mass or mass defect.

This can also be written as

$$E_e = \frac{\hbar c}{\lambda\!\!\!^{-}_{comp}} \left(1 - \frac{1}{\gamma}\right)$$

or

$$E_e = \frac{\hbar c}{\lambda\!\!\!^{-}_{comp}} - \frac{\hbar c}{\lambda\!\!\!^{-}_{comp}\gamma} \tag{3}$$

The change in energy between atomic states can be written as a relativistic photon wavelength defect evaluated at the reduced Compton wavelength corresponding to the mass defect of Eq. 2.

Equations 2 and 3 and the results presented in Tables 4 and 5 make a strong case that the Dirac equation can be understood as a relativistic mass or wave defect equation.

Further equivalency of the Dirac solution can also be written in the form of a de Broglie wave as follows,

$$\text{Dirac}\,\gamma^2 = 1 + \left[\frac{Z\alpha}{n - j - ½ + \sqrt{(j + ½)^2 - Z^2\alpha^2}}\right]^2$$

The transition energy can be written

$$E_e = ½m_ec^2\left(1-\frac{1}{\gamma^2}\right)$$

or

$$E_e = \frac{\hbar^2}{2m_e\lambdabar_{comp}^2}\left(1-\frac{1}{\gamma^2}\right)$$

or

$$E_e = \frac{\hbar^2}{2m_e\lambdabar_{comp}^2} - \frac{\hbar^2}{2m_e\lambdabar_{comp}^2\gamma^2}$$

Either a photon form or de Broglie form are interchangeable with the power of $\gamma$ naturally agreeing with the power of the reduced Compton wavelength. The transition energy can be interchangeably written as a mass defect (Dirac equation), photon wavelength defect or de Broglie wavelength defect.

Using this methodology does not directly permit calculation of multi-electron fine-structure given the Dirac Equation depends on Z. However, the concept of using a relativistic wavelength defect discussed here will lead to calculation of the fine-structure energy splits for single and multi-electron atoms.

# 5. Calculating p, d, f, g and h, etc. Energy Splits using the Relativistic Wave Defect

The results of Section 4 demonstrating the idea of a wave defect and the principal spectral line results of Section 1 and detailed in Appendix A will lead to the derivation of a coulombic de Broglie wave methodology for calculating the fine-structure for single and multi-electron atoms.

In the case of hydrogen and other single electron atoms, when using the Dirac equation, the principal state is represented by the total angular momentum $J = \frac{1}{2}$. The p states in the case of hydrogen are represented by $J = \frac{1}{2}$ and $\frac{3}{2}$ with the principal "s" state and first "p" state being theoretically degenerate, both calculated as $J = ½$. In fact, the principal and first p state are not degenerate. It is well known that the Dirac equation predicts the principal state and the p state energy split, the difference between $J = \frac{1}{2}$ and $\frac{3}{2}$, not the absolute values of the non-degenerate principal and first p state which is currently the domain of Quantum Electrodynamics (QED) [6]. The non-degeneracy of the s and first p-state is attributed to the lamb shift corrections (which can have several different meanings) [6] and is not predicted by the Dirac equation. This is the accepted understanding but emphasizes that it is the $J =$ ½ and second or $J = \frac{3}{2}$ p-state energy difference that is calculated with the Dirac equation. Calculation of this energy split is the subject of this section and is identical to the calculated product of the Dirac equation with the exception that the derivation developed in this section can be extended to multi-electron fine-structure.

To write the relevant equation for the fine-structure energy splits, an equation must be introduced that will be discussed in more detail in Appendix A. The equation is in essence a new quantum relation, although not strictly speaking a traditional one. The reason for introducing this equation at this point is that Eq. 1 does not have an obvious wave-like structure for application of the results of Section 4, although it turns out that Eq. 1 does have an implicit wave-like structure.

Section 4 demonstrated that a special relativistic change in wavelength based on the linear velocity change corresponding to the transition energy will give the same result as the Dirac equation. The following equation is directly equivalent to Eq. 1 and can be used to calculate principal spectra transitions, unmodified by the results of Section 4. The equivalency between Eq. 1 and Eq. 4 will be demonstrated in detail in Appendix A establishing that the Rydberg-Ritz equation as represented by Eq. 1 has a quantum basis.

$$\lambda\!\!\!^{-}_e = \frac{\hbar}{\sqrt{2m_e I_e\, e}} + \left(\frac{x}{a}\right)\left(\frac{\hbar c}{E_{r_{\lambda\!\!\!^{-}comp}}}\right) \tag{4}$$

$$E_{r_{\lambda\!\!\!^{-}comp}} = \left(\frac{e^2}{4\pi\varepsilon_o \lambda\!\!\!^{-}_{comp}}\right)$$

A very interesting characteristic of Eq.4 is that the second term is a constant and is written as a phonon characteristic length based on a constant coulombic energy evaluated at the Compton wavelength. The equation is essentially a photon interacting with an electron or electron state represented by a de Broglie wave with the ground state the de Broglie wave evaluated at the Ionization energy. The Coulomb energy coupling with photon's or de Broglie waves appears repeatedly and will be discussed in more detail in Appendix A. Equation 4 also states that the change in binding energy is a constant regardless of the actual energy of interaction which is the same situation seen in the Compton effect for a photon and free electron interaction. Both Eq. 4 and the Compton effect indicate a constant change based on the Compton wavelength regardless of input. This will also be discussed and explored further in Appendix A including a derivation of Compton scattering using the Energy-Momentum equation and a combined photon and de Broglie wave.

Applying the results of Section 4, Eq. 4 can be modified through multiplication by a relativistic factor that will be labeled $\gamma_\Delta$. This multiplication will create a wave defect as discussed in Section 4.

$$\lambdabar_\Delta = \left[\frac{\hbar}{\sqrt{2m_e I_e\, e}} + \left(\frac{x}{a}\right)\left(\frac{\hbar c}{E_{r_{\lambdabar_{comp}}}}\right)\right]\gamma_\Delta \qquad (5)$$

This theoretically will result in the p, d, f, g, and h, (and so on) energy splits if the correct energy can be identified that gives a correct $\gamma_\Delta$ a priori. When this approach was first recognized it was purely theoretical given that such an energy may not exist.

The details of finding the correct energy will not be given, but it turns out that there is an energy giving the correct $\gamma_\Delta$, and it is completely consistent with the more global principles presented in this paper. The relativistic linear kinetic energy factor $\gamma_\Delta$ can be evaluated from the coulombic energy of the transition using

$$\gamma_\Delta = \frac{1}{\sqrt{1 - \frac{2E_c}{m_e c^2}}} \text{ evaluated at } E_c = \frac{e^2}{4\pi\varepsilon_o\, \lambdabar_e} \qquad (6)$$

with $\lambdabar_e$ the principal spectral line transition. The simple coulombic energy appears naturally again.

After some development, the final form for $\gamma_\Delta$ is

$$\gamma_\Delta = \frac{1}{\sqrt{1 - \left(\frac{a}{4S}\right)\left(\frac{2E_c}{m_e c^2}\right)}} \qquad (7)$$

with the energy corresponding to energy split $E_\Delta$ for the fine-structure as a function of $\lambdabar_\Delta$ evaluated as

$$E_\Delta = \frac{\hbar^2}{2m_e \lambdabar_\Delta^2} \qquad (8)$$

If S turns out to be a constant for the fine-structure of any electron in any atom, then this methodology can be used predictively.

The “4” in Eq.6 is a normalizing factor which makes S for the p energy split equal to one when maintaining the linear kinetic energy form. The constant $a$ is the electron number as defined in Section 1.

Table 6. shows the hydrogen principal state results and the results for S using the NIST database [1] and Eq. 7. Table 6 demonstrates that S is in fact a constant, almost exactly an integer constant suggesting fundamental validity of the approach. The values also follow a natural arithmetic progression.

**Table 6: H I (ev); S (Eq.7)**

| $p\left(E_{\left(\frac{3}{2}\right)}-E_{\left(\frac{1}{2}\right)}\right);\ d\left(E_{\left(\frac{5}{2}\right)}-E_{\left(\frac{3}{2}\right)}\right);\ f\left(E_{\left(\frac{7}{2}\right)}-E_{\left(\frac{5}{2}\right)}\right)$; etc. | | | | | | |
|---|---|---|---|---|---|---|
| **n** | **2s** | **3s** | **4s** | **5s** | **6s** | |
| $E_n$ **(ev)** | **10.19791879** | **12.08695976** | **12.74819214** | **13.05426487** | **13.22053220** | |
| **NIST** | **10.19881044** | **12.08749486** | **12.74853289** | **13.05449835** | **13.22070151** | |
| **Δ%** | **8.74E-03** | **4.43E-3** | **2.67E-3** | **1.79E-3** | **1.28E-03** | |
| $E_e$ **(ev)** | **3.400515695** | **1.511474726** | **0.8502423419** | **0.5441696181** | **0.3779022902** | **S** |
| **S Calc.** | **2p** | **3p** | **4p** | **5p** | **6p** | |
| | **0.9978119708** | **0.997939608** | **0.998026562** | **0.9978091436** | **0.9980653593** | **1** |
| | | **3d** | **4d** | **5d** | **6d** | |
| | $S_p+2$ | **2.994157487** | **2.995556122** | **2.995268032** | **2.994860048** | **3** |
| | | | **4f** | **5f** | **6f** | |
| | | $S_d+3$ | **6.005091586** | **6.047301226** | **5.988491964** | **6** |
| | | | | **5g** | **6g** | |
| | | | $S_f+4$ | **9.980449447** | **9.980713037** | **10** |
| | | | | | **6h** | |
| | | | | $S_g+5$ | **15.97066886** | **15** |

Table 6 establishes the value for S and Table 7 presents the calculated results for hydrogen a priori using S. The percent difference between calculation using Eq. 7 and the NIST database is presented. The accuracy is very good.

When applied to multi-electron atoms, it turns out that the results hold for at least the inner 3 electrons for any atom, with the inner 1st and 3rd in very close agreement and the 2nd not quite as good but still very good accuracy. The close agreement of the 1st and 3rd, but slightly different 2nd, may be a meaningful result given that the 1st and 3rd electron are the first electron in a period and the 2nd should be different in character, being it is the 2nd electron in a period. It is possible that for any atom and the same electron number, such as the inner 4th or 10th, etc. that a specific S exists. It is also possible that there may be a consistent S for the 2nd electron of a period and the 3rd and so on. Unfortunately, the data is relatively sparse in these cases, but sufficient data exists for the inner 3 electrons of a sufficient number of atoms to demonstrate this uniformity and the correspondence between the all 1st and 3rd inner electrons and all 2nd inner electrons.  Additional results for multi-electron cases supporting these statements are presented in Appendix C.

**Table 7:  H I (ev); $E_{\Delta}$ (Eq. 7)**

| $p\left(E_{\left(\frac{3}{2}\right)}-E_{\left(\frac{1}{2}\right)}\right)$; $d\left(E_{\left(\frac{5}{2}\right)}-E_{\left(\frac{3}{2}\right)}\right)$; $f\left(E_{\left(\frac{7}{2}\right)}-E_{\left(\frac{5}{2}\right)}\right)$; etc.<br>$I_e = 13.509434486\ ev$ | | | | | |
|---|---|---|---|---|---|
| **n** | **2s** | **3s** | **4s** | **5s** | **6s** |
| **NIST** | **10.19881044** | **12.08749486** | **12.74853289** | **13.05449835** | **13.22070151** |
| **Eq. A.10** | **3.400515695** | **1.511474726** | **0.8502423419** | **0.5441696181** | **0.3779022902** |
| $E_n$ **(ev)** | **10.19791879** | **12.08695976** | **12.74819214** | **13.05426487** | **13.22053220** |
| **Δ%** | **0.00874%** | **0.00443%** | **0.00267%** | **0.00179%** | **0.00128%** |
| **S=1** | **2p** | **3p** | **4p** | **5p** | **6p** |
| **NIST** | **4.536434E-5** | **1.34413E-5** | **5.67042E-6** | **2.904E-6** | **1.68016E-6** |
| **Eq. B.5.** | **4.526458E-5** | **1.34135E-5** | **5.65726E-6** | **2.898E-6** | **1.67687E-6** |
| **Δ%** | **0.22%** | **0.21%** | **0.23%** | **0.21%** | **0.20%** |
| **S=3** | | **3d** | **4d** | **5d** | **6d** |
| **NIST** | | **4.4799E-6** | **1.8892E-6** | **9.674E-7** | **5.5993E-7** |
| **Eq. B.5.** | | **4.4712E-6** | **1.8864E-6** | **9.659E-7** | **5.5893E-7** |
| **Δ%** | | **0.19%** | **0.15%** | **0.16%** | **0.18%** |
| **S=6** | | | **4f** | **5f** | **6f** |
| **NIST** | | | **9.424E-7** | **4.7916E-7** | **2.80022E-7** |
| **Eq. B.5.** | | | **9.432E-7** | **4.8292E-7** | **2.79440E-7** |
| **Δ%** | | | **0.085%** | **0.78%** | **0.20%** |
| **S=10** | | | | **5g** | **6g** |
| **NIST** | | | | **2.9033E-7** | **1.68015E-7** |
| **Eq. B.5.** | | | | **2.8975E-7** | **1.67647E-7** |
| **Δ%** | | | | **0.20%** | **0.22%** |
| **S=15** | | | | | **6h** |
| **NIST** | | | | | **1.12013E-7** |
| **Eq. B.5.** | | | | | **1.11750E-7** |
| **Δ%** | | | | | **0.24%** |

# 6.  Conclusion

The initial purpose of this paper was to validate principles and relationships discovered in previous work (unpublished) through application to a very definitive case (atomic spectra) for comparison with accurate and available data (NIST database).  As the title indicates, this work can be summarized as an interrelationship between the de Broglie wave, the Coulomb potential and special relativity applied to a new quantum relation.

Several key results emerge in a consistent and quite natural way.

For example, Eq. (1) presented in Section 1 and derived in Appendix A, emerges as a Rydberg-Ritz type equation in a natural and unexpected way. There is nothing about the development and derivation that suggested at the outset that this would be the result. The result demonstrates that the Rydberg-Ritz equation has a quantum basis.

Throughout the paper, fundamental algebraic length relationships play a significant role. Three fundamental forms consistently emerge: the de Broglie wave; the photon; and the coulomb potential. The fundamental interactions occur between the lengths/wavelengths with the energy appearing as a result of the interaction.

The fine-structure of the atom emerges as a special relativistic mass defect or wave defect applied to the principal state quantum algebraic wavelength relation, Eq. 4, which itself is equivalent to Eq. 1 (see Appendix A). This is supported by the Dirac equation.

Example results for single and multi-electron principal and fine-structure spectra are presented in the main body of this paper. Additional results are presented in Appendix B and C.

The general accuracy of the principal spectra and fine-structure energy splits for single and multi-electron cases compared to the NIST database supports the general validity of the concepts. There are other unpublished applications where these same concepts have also led to excellent and tractable results, but it was first necessary to establish a very clear case for this, which, it is submitted, has been accomplished in this paper.

# 7. References

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# 8. Acknowledgement

The authors would like to thank Dr. Cynthia Powell, formerly Research Director, National Energy Technology Laboratory and currently at the Pacific Northwest National Laboratory for her unwavering support and encouragement in the pursuit of this work.

# 9. Disclaimer

# 10. Appendix A

The derivation of Eq. (1) along with additional observations and considerations applicable to its use and validity will be discussed.

## A.1. A Preliminary Semi-Classical Result

First, the simple development of a semi-classical equation is required. In this sub-section and throughout, certain assumptions will be made and assembled with the result of this process judged valid or in-valid based on utility in comparison to NIST measured principal spectral lines [4] for hydrogen without concern for the perceived a priori validity of the assumptions. Units of electron volts are used.

It is assumed that for any electron, any atom.

$$E_{spectra} = E_o - E_e \qquad (A.1)$$

$E_o$ and $E_e$ are unknown with $E_{spectra}$ representing the principal spectral line energy for any electron, any atom, for the transition between the ground state and the n^th principal excited state. It will be assumed that $E_o$ is the Ionization Energy $(I_e)$ since in the sense of a binding energy determined from the mass defect for a proton and electron, the binding energy is virtually equal to the Ionization Energy of atomic hydrogen. It remains to determine a general relation for an electron transition energy $E_e$.

It will be assumed that $E_e$ represents the energy of a non-specific electron state and can be evaluated as a de Broglie energy,

$$E_e = \frac{\hbar^2}{(2m_e\,\lambda\!\!\!^{-}{}_e^2\,)e}$$

The de Broglie energy is evaluated as a function of the Coulombic characteristic length $r$ which itself is evaluated at the Ionization Energy.

$$r = \frac{e}{4\pi\varepsilon_o I_e}$$

Arbitrarily, at this point, the function of r chosen is given by $\lambda\!\!\!^{-}_e = ½r$, with $\lambda\!\!\!^{-}_e$ representing the de Broglie wavelength of a general electron state. There is a theoretical reason that $\lambda\!\!\!^{-}_e = ½r$ is selected, but this will not be addressed here to keep the development moving along. These assumptions, and for what are at this point arbitrary considerations, leads to,

$$E_e = \frac{\hbar^2}{\left(2m_e\left(\frac{r}{2}\right)^2\right)e}$$

which results in,

$$E_e = \left(\frac{32\pi^2\varepsilon_o^2\hbar^2 I_e^2}{m_e e^3}\right) = \frac{I_e^2}{R_\infty} \qquad (A.2)$$

In these equations, $R_\infty$ represents $(R_\infty hc)/e = 13.60569253\ (ev)$.

To calculate the spectra for any transition, any electron, in any atom with Eq. A.2, $Z_{eff}$ and $n$ must be inserted artificially, which does not fundamentally improve things compared to existing methods. (However, $Z_{eff}, n$ and $R_\infty$ will drop out naturally, as the development proceeds, after which, R∞ will reemerge ($Z_{eff}$ and $n$ drop out permanently) in a form expected for the Ritz equation). This results in,

$$E_{spectra} = I_e - \left(\frac{I_e^2}{Z_{eff}^2\, n^2\, R_\infty}\right) \qquad (A.3)$$

The semi-classical Eq. A.3, while not particularly useful, is a preliminary and new result that will have use in the development that follows. It is very distinct from the Bohr equation and it is the precursor to results that will have stand-alone utility. The results discussed in the next section will have an unexpected relationship to the Dirac equation. This relationship is discussed in Appendix B.

## A.2. Interaction of the Bound State with a Photon

The assumptions and developments contained in this section are independent of Section A.1, resulting in two distinct equations for calculating the same result, which when combined, results in an equation of the form of the Rydberg-Ritz Combination principle. This combined result can be used explicitly to calculate principal spectral lines without the need for a $Z_{eff}$ or a quantum defect or any fitted parameter.

A second relationship for atomic bound state transitions can be written that is directly related to Compton scattering for a radiation interaction with a 'free' electron. The key characteristic of Compton scattering to be applied is that the Compton wavelength represents a constant change in radiation wavelength, when a photon interacts with an electron, regardless of the wavelength of the input radiation.

In this section, it will be assumed that the wavelength of the ground state of an electron can be represented by the de Broglie wave evaluated at the Ionization Energy of the electron for any electron, any atom.

$$E_o = atomic\ ground\ state = I_e$$

$$ƛ_o = \frac{\hbar}{\sqrt{2m_e I_e e}} \qquad (A.4)$$

It will be assumed that for a bound electron the change of the electron state responding to a radiation input will be evaluated as a constant change in wavelength corresponding to the Bohr radius ($a_o$) in the same manner as the Compton effect for a "free" electron is constant in terms of the Compton wavelength.

The first principal state is equal to the ground state de Broglie wave, plus one Bohr radius. The second principal state is equal to the ground state plus two Bohr radii, and so on.

$$ƛ_e = ƛ_o + \left(\frac{x}{a}\right) a_o \qquad (A.5)$$

$x =$ the principal energy transition – 1st transition $x = 1$; 2nd transition $x = 2$; and so on

$a =$ the electron number. For the outer electron $a = 1$; $a$ ranges from Z to 1

$ƛ_e =$ the de Broglie wavelength of the excited principal state.

$ƛ_o =$ the de Broglie wavelength evaluated at the Ionization Energy of the electron state representing the ground state.

$a_o =$ the constant change in electron state wavelength, regardless of energy input. is equal to the Bohr radius.

To demonstrate the interaction between the electron state and photon as a type of wave/particle interaction, depending on interpretation, the Bohr radius and Compton wavelength can be related using the following identity,

$$\frac{E_{rad_{a_o}}}{E_{r_{\lambda_{comp}}}} = \frac{\frac{\hbar c}{a_o}}{\frac{e^2}{4\pi\varepsilon_o\lambda_{comp}}} = 1 \qquad (A.6)$$

permitting Eq. (A.5) to be rewritten as,

$$\boxed{\lambda_e = \frac{\hbar}{\sqrt{2m_e I_e\, e}} + \left(\frac{x}{a}\right)\left(\frac{\hbar c}{E_{r_{\lambda_{comp}}}}\right)} \qquad (4)$$

Equation 4 was first introduced in Section 4. as essential to the calculation of fine-structure.

The first term of Eq. 4 is generally considered a wave form and the second term is generally considered a particle form.

Equation A.5 and Eq. 4 are equivalent and general. Equation A.5 will be used for further development leading to the equation corresponding to the Rydberg-Ritz Combination Principle, but Eq. 4 establishes a relationship between the bound state and a radiation 'packet' evaluated at an energy dependent on the Compton wavelength. This algebraic and therefore intrinsically discrete interaction of the electron state and radiation as a wave/particle interaction explicitly defines an atomic electron transition as the algebraic addition of a photon to an electron state (or electron) in a natural way. In other words, the addition of a wave form and particle form reduces to the addition of two lengths.

Another implication of Eq. 4, that $\lambda_{comp}$ is fundamental to radiation interaction with a de Broglie wave, is that the constant $½m_ec^2$ in the Energy-Momentum equation can be written,

$$½m_ec^2 = \frac{\hbar c}{2\lambda_{comp}} = \frac{\hbar^2}{2m_e\lambda_{comp}^2}$$

or

$$m_ec^2 = \boxed{\frac{\hbar c}{2\lambda_{comp}} + \frac{\hbar^2}{2m_e\lambda_{comp}^2}} \qquad (A.8)$$

Either the de Broglie form or photon form or both can be substituted into the Energy-Momentum equation. The forms are interchangeable and demonstrates a type of interchangeable duality in that either individually or both can be concurrently substituted and simply added, giving the same result.

If Eq. A.8 is used and both are substituted concurrently, a derivation of Compton scattering follows (a prime means post-scattering),

$$E_e' = E_\gamma - E_\gamma' + m_e c^2 \qquad (Conservation\ of\ Energy)$$

$$p_e' = p_\gamma - p_\gamma' \qquad (Conservation\ of\ Momentum)$$

$$E_e' = \sqrt{(p_e' c)^2 + (m_e c^2)^2} \qquad (E\text{-}M\ Equation)$$

substitution of appropriate terms, including Eq. A.8, and rearranging,

$$p_e c^2 = \left(\frac{\hbar c}{\bar{\lambda}} + \boxed{\frac{\hbar c}{2\lambda_{comp}} + \frac{\hbar^2}{2m_e\bar{\lambda}_{comp}^2}} + \frac{\hbar c}{\bar{\lambda}'}\right)^2 - \boxed{\left(\frac{\hbar c}{2\lambda_{comp}} + \frac{\hbar^2}{2m_e\bar{\lambda}_{comp}^2}\right)^2} \qquad (A.9)$$

$$p_e c^2 = (p \cdot p)c^2 = \left(\frac{\hbar c}{\bar{\lambda}}\right)^2 + \left(\frac{\hbar c}{\bar{\lambda}'}\right)^2 - \frac{2\hbar^2 c^2}{\bar{\lambda}\bar{\lambda}'} cos\theta$$

setting these equal and simplifying,

$$\frac{\hbar^2 c^2}{\lambda_{comp}}\left(\frac{1}{\bar{\lambda}} - \frac{1}{\bar{\lambda}'}\right) + \frac{\hbar^3 c}{m_e\bar{\lambda}_{comp}^2}\left(\frac{1}{\bar{\lambda}} - \frac{1}{\bar{\lambda}'}\right) = \frac{2\hbar^2 c^2}{\bar{\lambda}\bar{\lambda}'}(1 - cos\theta)$$

$$½\frac{1}{\lambda_{comp}}\left(\frac{1}{\bar{\lambda}} - \frac{1}{\bar{\lambda}'}\right) + ½\left(\frac{\hbar}{m_e c}\right)\left(\frac{1}{\bar{\lambda}_{comp}^2}\right)\left(\frac{1}{\bar{\lambda}} - \frac{1}{\bar{\lambda}'}\right) = \frac{1}{\bar{\lambda}\bar{\lambda}'}\ (1 - cos\theta)$$

$$\frac{1}{\lambda_{comp}}\left(\frac{1}{\bar{\lambda}} - \frac{1}{\bar{\lambda}'}\right) = \frac{1}{\bar{\lambda}\bar{\lambda}'}(1 - cos\theta)$$

$$\bar{\lambda}' - \bar{\lambda} = \lambda_{comp}(1 - cos\theta) \qquad (Compton\ Scattering)$$

This demonstrates that at the Compton wavelength, the radiation or photon energy form or the de Broglie energy form are equivalent and strongly supports that they are in general additive as Eq. A.7 demonstrates when addressing the interaction of radiation with the bound state.

Given that the derivation of the Compton effect was developed based on one photon (not a wave-train) interacting with one ‘free’ electron, it suggests that the Compton wavelength could be thought of as a constant fundamental to the change in characteristic length of either a photon (Compton scattering) or electron Eq. A.7. In some respects, Compton scattering or Eq. A.7 represents a conservation of wavelength principle between a photon and electron.

## A.3. Eliminating the Effective Atomic Number or Quantum Defect

The next step is to develop a relationship for $Z_{eff}$ that will enable writing the simplest expression for the equation representing the Rydberg-Ritz Combination Principle.

Using the original assumption that an electron can be represented as a de Broglie wave and using Eq. A.5, the energy of the electron state for any electron, any atom, can be written,

$$E_e = \frac{\hbar^2}{2m_e \lambdabar_e^2} \qquad (A.10)$$

$$E_{spectra} = I_e - \frac{\hbar^2}{2m_e\left(\lambdabar_o + \frac{x}{a}a_o\right)^2} \qquad (A.11)$$

Equation A.11 can be used to calculate the principal spectral line for any electron, any atom, although this is still not the final form.

Substituting $E_e$ from Eq. A.2 into $\lambdabar_e$ of Eq. A.5,

$$\frac{\hbar}{\left(\frac{2m_e I_e^2}{Z_{eff}^2 n^2 R_\infty}\right)^{½}} = \frac{\hbar}{(2m_e I_e)^{½}} + \left(\frac{x}{a}\right)a_o$$

Rearranging,

$$Z_{eff} = \left(\frac{1}{n}\right)\left(\frac{I_e}{R_\infty}\right)^{½}\left(1 + \left(\frac{x}{a}\right)\left(\frac{a_o}{\lambda_o}\right)\right) \qquad (A.12)$$

Substituting Eq. A.12 into Eq. A.3 eliminates $Z_{eff,}$ $n$ and $R_\infty$ naturally, resulting in,

$$E_{spectra} = I_e - \frac{I_e}{\left(1 + \left(\frac{x}{a}\right)\left(\frac{a_o}{\lambdabar_o}\right)\right)^2} \qquad (A.13)$$

Using Eq. A.13, any principal spectra can be calculated for any electron and for any atom, single or multi-electron, using the correct value of x and a. It is important to note that a positive energy frame of reference is used which is the natural frame for this analysis. Electron states lose energy (wavelength or characteristic length of the electron state becomes longer) as the transition number increases.

## A.4. A New Rydberg-Ritz Equation

The following result from Section A.2.

$$\tfrac{1}{2} m_e c^2 = \frac{\hbar^2}{2 m_e \bar{\lambda}_{comp}^2}$$

is equivalent to the identity,

$$\left(\frac{I_e}{R_\infty}\right)^{1/2} = \frac{a_0}{\bar{\lambda}_o} \qquad (A.14)$$

and substituting A. 14 into Eq. A.13 results in,

$$\boxed{E_{spectra} = I_e - \frac{I_e R_\infty}{\left(\sqrt{R_\infty} + \left(\frac{x}{a}\right)\sqrt{I_e}\right)^2}} \qquad (1)$$

which has the identical form of the Rydberg-Ritz equation typically written as,[2]

$$T = A - \frac{(Z - \delta_o)^2 R_\infty}{(m + a)^2}$$

where A is empirically determined to be the Ionization Potential and $(Z - \delta_o)$ is essentially a $Z_{eff}$ or more commonly referred to as the quantum defect. The Rydberg-Ritz equation is currently used to fit some of the spectral data in the National Institute of Standards and Technology (NIST) database.[1]

## A.5. Two Equivalent Calculations

Calculations for the first hydrogen transition using Eq. A.13 and Eq. 1 demonstrate that despite their very different appearance they give the same result.

Using Eq. A.13,

$I_e = 13.598434486\ ev$

$m_e = 9.10938291E\text{-}31\ kg$

$a_o = \dfrac{4\pi\varepsilon_o\ \hbar^2}{m_e\ e^2} = 5.2917721092E\text{-}11\ m$

$\lambda\!\!\!^{-}_o = \dfrac{\hbar}{\sqrt{2m_e I_e e}} = 5.293184138E\text{-}11\ m$

$$E_{spectra} = I_e - \frac{I_e}{\left(1 + \left(\frac{x}{a}\right)\left(\frac{a_o}{\lambda\!\!\!^{-}_o}\right)\right)^2} \tag{A.13}$$

$$E\_spectra\ (H) = 13.598434486 - \frac{13.598434486}{\left(1 + \left(\frac{1}{1}\right)\left(\frac{5.2917721092E\text{-}11}{5.293184138E\text{-}11}\right)\right)^2}$$

$$E_{spectra}(H\ I) = 10.19791879\ eV$$

Using equation A.1,

$I_e = 13.598434486\ ev$

$R_\infty = 13.60560253$

$$E_{spectra} = I_e - \frac{R_\mu I_e}{\left(\sqrt{R_\mu} + \left(\frac{x}{a}\right)\sqrt{I_e}\right)^2} \tag{1}$$

$$E_{spectra}\ \ (H) = 13.598434486 - \frac{(13.60569253)(13.5984344869)}{\left(\left(\sqrt{13.60569253} + \left(\frac{1}{1}\right)\sqrt{13.598434486}\right)\right)^2}$$

$$E_{spectr}(H\ I) = 10.19791879\ eV$$

## A.6. Conclusion

The derivation of the equation for Compton scattering from the Energy-Momentum equation using an additive photon and de Broglie wave indicates the compatibility and interchangeability of the two physical entities. Appendix A details additional examples of this algebraic compatibility between physical entities that may not be a priori considered interchangeable, but are.

A first key principle is application of the Compton scattering result to the bound state that the change in wavelength is constant (Compton wavelength) regardless of input. This principle emerges in the interaction of the photon with a bound electron state and leads to calculation of the principal energy spectra and ultimately Eq. 1.

A second key principle is that the Coulomb energy is an implicit part of both the de Broglie wave (Eq. A.2) and the photon (Eq. 4). Essentially a coulombic de Broglie wave or a coulombic photon results. In the first case, the Coulomb energy is the energy term of the semi-classical result, and in the second, it is the energy term of a quantum result. The combination of the semi-classical and quantum result leads to Eq. 1 calculation of the principal spectra. Combination of the quantum and special relativistic result (Eq.5) leads to calculation of fine-structure.

# 11. Appendix B - Multi-Electron Results for Principal Spectral Lines

Calculations using Eq. (1) are presented for multi-electron atoms (with a few single electron results included). The criteria for selection was based on including representative Periods where adequate data existed in the NIST database. It should be noted that data does not exist for most electrons and when it does exist, it is usually limited to a few transitions. In some cases, such as Ba I, Cs II and Fr II, data for a large number of transitions does exist providing a good comparison of results where trends can be identified. Another consideration is a focus on the first electron in a period where the principal spectral line can be very clearly identified. As more electrons fill the period, it becomes increasingly unclear what is a principal spectral line (of course the Dirac equation $J = ½$ does not help for multi-electron cases). Some calculations were done for cases that include more than one electron in a period with the resulting accuracy well within reasonable limits, but, in fact, it was impossible to determine if the error was relative to a principal spectral line or due to the inability to identify a principal spectral line so they are not included due to ambiguity. Calculations are therefore presented for the first electron of a period where ambiguity did not exist. These calculations are presented in Tables B.1 through B.26.

In the case of the first transition of the principal spectral lines, the Eq. (1) accuracy is on the order of 0.1% for multi-electron Period 2 light elements and on the order of at most 2 to 4% for multi-electron Period 6 & 7 elements including the francium valence electron. The accuracy in virtually all cases improves dramatically from this result for the first transition as transition number increases. There is no divergence at higher transition numbers, but very strong convergence, which is somewhat remarkable given the lines become increasingly closer and harder to separate as the transition number increases.

All energy values are in electron volts.

## Second Period

### Table B.1: Li I

| Li | Z | | a | |
|---|---|---|---|---|
| 1 | 3 | | 1 | |
| **Configuration** | **NIST (eV)** | **X** | **Equation (1)** | **Δ%** |
| $1s^2 2s$ | 0.0000000 | | | |
| $1s^2 3s$ | 3.3731290 | 1 | 3.3613130 | 0.35030 |
| $1s^2 4s$ | 4.3409420 | 2 | 4.3352811 | 0.13041 |
| $1s^2 5s$ | 4.7485330 | 3 | 4.7455834 | 0.06212 |
| $1s^2 6s$ | 4.9578350 | 4 | 4.9561346 | 0.03430 |
| $1s^2 7s$ | 5.0793700 | 5 | 5.0783264 | 0.02055 |
| $1s^2 8s$ | 5.1561400 | 6 | 5.1554809 | 0.01278 |
| $1s^2 9s$ | 5.2077500 | 7 | 5.2072906 | 0.00882 |
| $1s^2 10s$ | 5.2443000 | 8 | 5.2437529 | 0.01043 |
| $1s^2 11s$ | 5.2706000 | 9 | 5.2703811 | 0.00415 |
| **Li I IP** | 5.3917150 | | | |

### Table B.2: C IV

| C | Z | Rμ | a | |
|---|---|---|---|---|
| 4 | 6 | 13.60445788 | 4 | |
| **Configuration** | **NIST (eV)** | **X** | **Equation (1)** | **Δ%** |
| $1s^2 2s$ | 0.0000000 | | | |
| $1s^2 3s$ | 37.5484900 | 1 | 37.4514908 | 0.25833 |
| $1s^2 4s$ | 49.7608200 | 2 | 49.7097353 | 0.10266 |
| $1s^2 5s$ | 55.2186600 | 3 | 55.1905062 | 0.05099 |
| $1s^2 6s$ | 58.1218100 | 4 | 58.1049920 | 0.02894 |
| $1s^2 7s$ | 59.8479200 | 5 | 59.8371004 | 0.01808 |
| $1s^2 8s$ | 60.9569300 | 6 | 60.9495841 | 0.01205 |
| $1s^2 9s$ | 61.7114900 | 7 | 61.7062591 | 0.00848 |
| **C IV IP** | 64.4935200 | | | |

## Table B.3:  N V

| N | Z |  | a |  |
|---|---|---|---|---|
| 5 | 7 |  | 5 |  |
| **Configuration** | **NIST (eV)** | **X** | **Equation (1)** | **Δ%** |
| $1s^2 2s$ | 0.00000 |  |  |  |
| $1s^2 3s$ | 56.55249 | 1 | 56.4249766 | 0.22548 |
| $1s^2 4s$ | 75.17767 | 2 | 75.1100981 | 0.08988 |
| $1s^2 5s$ | 83.55124 | 3 | 83.5140350 | 0.04453 |
| $1s^2 6s$ | 88.02124 | 4 | 87.9991403 | 0.02511 |
| $1s^2 7s$ | 90.68519 | 5 | 90.6712008 | 0.01543 |
| $1s^2 8s$ | 92.39992 | 6 | 92.3904173 | 0.01028 |
| $1s^2 9s$ | 93.56802 | 7 | 93.5613332 | 0.00715 |
| $1s^2 10s$ | 94.39942 | 8 | 94.3945420 | 0.00517 |
| N V IP | 97.89014 |  |  |  |

## Table B.4:  O VI

| O | Z |  | a |  |
|---|---|---|---|---|
| 6 | 8 |  | 6 |  |
| **Configuration** | **NIST (eV)** | **X** | **Equation (1)** | **Δ%** |
| $1s^2 2s$ | 0.0000000 |  |  |  |
| $1s^2 3s$ | 79.3548200 | 1 | 79.1967907 | 0.19914 |
| $1s^2 4s$ | 105.7208000 | 2 | 105.6371447 | 0.07913 |
| $1s^2 5s$ | 117.6230000 | 3 | 117.5786947 | 0.03767 |
| $1s^2 6s$ | 123.9940000 | 4 | 123.9680299 | 0.02094 |
| $1s^2 7s$ | 127.8000000 | 5 | 127.7811231 | 0.01477 |
| $1s^2 8s$ | 130.2507000 | 6 | 130.2375426 | 0.01010 |
| O VI IP | 138.1189000 |  |  |  |

## Table B.5: F VII

| F | Z | | a | |
|---|---|---|---|---|
| 7 | 9 | | 7 | |
| **Configuration** | **NIST (eV)** | **X** | **Equation (1)** | **Δ%** |
| $1s^2 2s$ | 0.00000 | | | |
| $1s^2 3s$ | 105.95950 | 1 | 105.7726280 | 0.17636 |
| $1s^2 4s$ | 141.39550 | 2 | 141.2974970 | 0.06931 |
| $1s^2 5s$ | 157.44520 | 3 | 157.3913456 | 0.03421 |
| $1s^2 6s$ | 166.05070 | 4 | 166.0186012 | 0.01933 |
| $1s^2 7s$ | 171.19430 | 5 | 171.1738391 | 0.01195 |
| F VII IP | 185.18680 | | | |

## Fourth Period

## Table B.6: Fe XXIV

| Fe | Z | | a | |
|---|---|---|---|---|
| 24 | 26 | | 24 | |
| **Configuration** | **NIST (eV)** | **X** | **Equation (1)** | **Δ%** |
| $1s^2 2s$ | 0.00000 | | | |
| $1s^2 3s$ | 1149.64300 | 1 | 1149.6381437 | 0.00042 |
| $1s^2 4s$ | 1545.38900 | 2 | 1545.3172772 | 0.00464 |
| $1s^2 5s$ | 1726.53570 | 3 | 1726.8567799 | 0.01860 |
| Fe XXIV IP | 2045.75900 | | | |

## Table B.7: Fe XVI

| Fe | Z | | a | |
|---|---|---|---|---|
| 16 | 26 | | 16 | |
| **Configuration** | **NIST (eV)** | **X** | **Equation (1)** | **Δ%** |
| $2p^6 3s$ | 0.00000 | | | |
| $2p^6 4s$ | 231.57020 | 1 | 230.4327577 | 0.49119 |
| $2p^6 5s$ | 330.05000 | 2 | 329.4691354 | 0.17599 |
| $2p^6 6s$ | 381.38000 | 3 | 380.8956802 | 0.12699 |
| $2p^6 7s$ | 412.00000 | 4 | 410.9757570 | 0.24860 |
| Fe XVI IP | 489.31200 | | | |

## Table B.8: Cu XXVIX

| Cu | Z | | a | |
|---|---|---|---|---|
| 29 | 29 | | 29 | |
| **Configuration** | **NIST (eV)** | **X** | **Equation (1)** | **Δ%** |
| 1s | 0.000 | | | |
| 2s | 8666.838 | 1 | 8691.454 | 0.28403 |
| 3s | 10281.955 | 2 | 10291.640 | 0.09419 |
| 4s | 10845.942 | 3 | 10850.529 | 0.04230 |
| 5s | 11106.427 | 4 | 11108.929 | 0.02253 |
| Cu XXIX IP | 11567.613 | | | |

## Table B.9: Cu XXVII

| Cu | Z | | a | |
|---|---|---|---|---|
| 27 | 29 | | 27 | |
| **Configuration** | **NIST (eV)** | **X** | **Equation (1)** | **Δ%** |
| 2s | 0 | | | |
| 3s | 1452.398 | 1 | 1453.440981 | 0.07181097 |
| 4s | 1952.9668 | 2 | 1953.849193 | 0.045182188 |
| 5s | 2182.891 | 3 | 2183.478903 | 0.026932323 |
| Cu XXVII IP | 2586.954 | | | |

## Table B.10: Cu XIX

| Cu | Z | | a | |
|---|---|---|---|---|
| 19 | 29 | | 19 | |
| **Configuration** | **NIST (eV)** | **X** | **Equation (1)** | **Δ%** |
| 3s | 0 | | | |
| 4s | 314.3545 | 1 | 313.0559918 | 0.413071295 |
| Cu XIX IP | | | | |

# Table B.11: Cu I

| Cu<br>1 | Z<br>29 | | a<br>1 | |
|---|---|---|---|---|
| **Configuration** | **NIST (eV)** | **X** | **Equation (1)** | **Δ%** |
| $d^{10}4s$ | 0.00 | | | |
| $d^{10}5s$ | 5.3483347 | 1 | 5.2101096 | 2.58445 |
| $3d^{10}6s$ | 6.5524100 | 2 | 6.4929944 | 0.90677 |
| $3d^{10}7s$ | 7.0263552 | 3 | 6.9953249 | 0.44163 |
| $3d^{10}8s$ | 7.2616180 | 4 | 7.2424841 | 0.26349 |
| $3d^{10}9s$ | 7.3953930 | 5 | 7.3820376 | 0.18059 |
| $3d^{10}20s$ | 7.6815300 | 16 | 7.6765545 | 0.06477 |
| $3d^{10}21s$ | 7.6862500 | 17 | 7.6813647 | 0.06356 |
| $3d^{10}22s$ | 7.6902600 | 18 | 7.6854478 | 0.06258 |
| $3d^{10}23s$ | 7.6937200 | 19 | 7.6889432 | 0.06209 |
| $3d^{10}24s$ | 7.6966850 | 20 | 7.6919585 | 0.06141 |
| $3d^{10}25s$ | 7.6992800 | 21 | 7.6945779 | 0.06107 |
| $3d^{10}26s$ | 7.7015710 | 22 | 7.6968677 | 0.06107 |
| $3d^{10}27s$ | 7.7035200 | 23 | 7.6988809 | 0.06022 |
| $3d^{10}28s$ | 7.7052990 | 24 | 7.7006604 | 0.06020 |
| $3d^{10}29s$ | 7.7068520 | 25 | 7.7022410 | 0.05983 |
| $3d^{10}30s$ | 7.7082700 | 26 | 7.7036513 | 0.05992 |
| $3d^{10}31s$ | 7.7095210 | 27 | 7.7049149 | 0.05975 |
| $3d^{10}32s$ | 7.7106470 | 28 | 7.7060515 | 0.05960 |
| $3d^{10}33s$ | 7.7116600 | 29 | 7.7070775 | 0.05942 |
| $3d^{10}34s$ | 7.7125940 | 30 | 7.7080068 | 0.05948 |
| $3d^{10}35s$ | 7.7134200 | 31 | 7.7088512 | 0.05923 |
| $3d^{10}36s$ | 7.7142000 | 32 | 7.7096207 | 0.05936 |
| $3d^{10}37s$ | 7.7148500 | 33 | 7.7103240 | 0.05867 |
| $3d^{10}38s$ | 7.7155100 | 34 | 7.7109684 | 0.05886 |
| $3d^{10}39s$ | 7.7160900 | 35 | 7.7115603 | 0.05870 |
| $3d^{10}40s$ | 7.7166200 | 36 | 7.7121053 | 0.05851 |
| $3d^{10}41s$ | 7.7171200 | 37 | 7.7126082 | 0.05846 |
| **Cu I IP** | 7.7218700 | | | |

## Fifth Period

### Table B.12: Cs LV

| Cs<br>55 | Z<br>55 | | a<br>55 | |
|---|---|---|---|---|
| **Configuration** | **NIST (eV)** | **X** | **Equation (1)** | |
| 1*s* | 0 | | | |
| 2*s* | 32064.58 | 1 | 32407.70424 | 1.070103641 |
| 3*s* | 38142.88 | 2 | 38276.31978 | 0.349841908 |
| Cs LV IP | 42912.99 | | | |

### Table B.13: Cs LIII

| Cs<br>53 | Z<br>55 | | a<br>53 | |
|---|---|---|---|---|
| **Configuration** | **NIST (eV)** | **X** | **Equation (1)** | **Δ%** |
| 2*s* | 0 | | | |
| 3*s* | 5752.7 | 1 | 5771.707674 | 0.330413092 |
| 4*s* | 7734.4 | 2 | 7740.400652 | 0.077583933 |
| 5*s* | 8641.1 | 3 | 8639.428169 | 0.019347437 |
| Cs LIII IP | 10208.78 | | | |

### Table B.14: Cs XLV

| Cs<br>45 | Z<br>55 | | a<br>45 | |
|---|---|---|---|---|
| **Configuration** | **NIST (eV)** | **X** | **Equation (1)** | **Δ%** |
| 3*s* | 0 | | | |
| 4*s* | 1588.99 | 1 | 1588.715537 | 0.017272788 |
| 5*s* | 2295.21 | 2 | 2295.008322 | 0.008786905 |
| 6*s* | 2668.7 | 3 | 2669.292047 | 0.022184855 |
| Cs XLV IP | 3485 | | | |

### Table B.15: Cs XXVII

| Cs<br>27 | Z<br>55 | | a<br>27 | |
|---|---|---|---|---|
| **Configuration** | **NIST (eV)** | **X** | **Equation (1)** | **Δ%** |
| 4*s* | 0 | | | |
| 5*s* | 380.72 | 1 | 377.277716 | 0.904151091 |
| Cs XXVII IP | 916.1 | | | |

## Table B.16: Cs IX

| Cs<br>9 | Z<br>55 | | a<br>9 | |
|---|---|---|---|---|
| **Configuration** | **NIST (eV)** | **X** | **Equation (1)** | **Δ%** |
| $4d^{10}5s$ | 0 | | | |
| $4d^{10}6s$ | 56.8737 | 1 | 55.40514274 | 2.582137717 |
| $4d^{10}7s$ | 81.8689 | 2 | 80.85066297 | 1.243740948 |
| $4d^{10}8s$ | 95.268 | 3 | 94.60627133 | 0.694596996 |
| $4d^{10}9s$ | 103.402 | 4 | 102.8731479 | 0.511452445 |
| Cs IX IP | 125.61 | | | |

## Table B.17: Cs I

| Cs<br>1 | Z<br>55 | | a<br>1 | |
|---|---|---|---|---|
| **Configuration** | **NIST (eV)** | **X** | **Equation (1)** | **Δ%** |
| $5p^6 6s$ | 0.0000000 | | | |
| $5p^6 7s$ | 2.2981126 | 1 | 2.2412511 | 2.47427 |
| $5p^6 8s$ | 3.0149423 | 2 | 2.9851134 | 0.98937 |
| $5p^6 9s$ | 3.3364969 | 3 | 3.3200619 | 0.49258 |
| $5p^6 10s$ | 3.5087811 | 4 | 3.4989464 | 0.28029 |
| $5p^6 11s$ | 3.6118742 | 5 | 3.6055698 | 0.17455 |
| $5p^6 12s$ | 3.6784628 | 6 | 3.6741953 | 0.11601 |
| $5p^6 13s$ | 3.7239631 | 7 | 3.7209466 | 0.08100 |
| $5p^6 14s$ | 3.7564292 | 8 | 3.7542210 | 0.05878 |
| $5p^6 15s$ | 3.7804051 | 9 | 3.7787414 | 0.04401 |
| $5p^6 16s$ | 3.7986133 | 10 | 3.7973294 | 0.03380 |
| $5p^6 17s$ | 3.8127663 | 11 | 3.8117552 | 0.02652 |
| $5p^6 18s$ | 3.8239848 | 12 | 3.8231745 | 0.02119 |
| $5p^6 19s$ | 3.8330276 | 13 | 3.8323684 | 0.01720 |
| $5p^6 20s$ | 3.8404230 | 14 | 3.8398795 | 0.01415 |
| $5p^6 21s$ | 3.8465482 | 15 | 3.8460950 | 0.01178 |
| $5p^6 22s$ | 3.8516783 | 16 | 3.8512964 | 0.00991 |
| $5p^6 23s$ | 3.8560177 | 17 | 3.8556930 | 0.00842 |
| $5p^6 24s$ | 3.8597210 | 18 | 3.8594426 | 0.00721 |
| $5p^6 25s$ | 3.8629068 | 19 | 3.8626663 | 0.00623 |
| Cs I IP | 3.8939057 | 9.109292709E-31 | | |

### Table B.18: Ba LVI

| Ba<br>56 | Z<br>56 | 13.60556021 | a<br>56 | |
|---|---|---|---|---|
| **Configuration** | **NIST (eV)** | **X** | **Equation (1)** | **Δ%** |
| 1*s* | 0 | | | |
| 2*s* | 33291.52 | 1 | 33661.76414 | 1.112127486 |
| 3*s* | 39607.93 | 2 | 39752.04057 | 0.363842711 |
| Ba LVI IP | 44561.47 | | | |

### Table B.19: Ba LIV

| Ba<br>54 | Z<br>56 | | a<br>54 | |
|---|---|---|---|---|
| **Configuration** | **NIST (eV)** | **X** | **Equation (1)** | **Δ%** |
| 2s | 0 | | | |
| 3s | 5984.296 | 1 | 6004.955576 | 0.345229849 |
| 4s | 8045.099 | 2 | 8051.785325 | 0.083110534 |
| 5s | 8987.8 | 3 | 8986.158157 | 0.018267461 |
| Ba LIV IP | 10616.42 | | | |

### Table B.20: Ba XLVI

| Ba<br>46 | Z<br>56 | | a<br>46 | |
|---|---|---|---|---|
| **Configuration** | **NIST (eV)** | **X** | **Equation (1)** | **Δ%** |
| 3s | 0 | | | |
| 4s | 1659.59 | 1 | 1659.145921 | 0.026758371 |
| 5s | 2397.4 | 2 | 2396.853327 | 0.022802734 |
| 6s | 2787.7 | 3 | 2787.817797 | 0.004225595 |
| Ba XLVII IP | 3640 | | | |

### Table B.21: Ba XXVIII

| Ba<br>28 | Z<br>56 | | a<br>28 | |
|---|---|---|---|---|
| **Configuration** | **NIST (eV)** | **X** | **Equation (1)** | **Δ%** |
| 4s | 0 | | | |
| 5s | 404.62 | 1 | 401.0291837 | 0.887453987 |
| Ba XXIX IP | 976.62 | | | |

## Table B.22: Ba X

| Ba | Z | | a | |
|---|---|---|---|---|
| 10 | 56 | | 10 | |
| **Configuration** | **NIST (eV)** | **X** | **Equation (1)** | **Δ%** |
| 5s | 0 | | | |
| 6s | 65.1051 | 1 | 63.46032086 | 2.526344536 |
| 7s | 94.2824 | 2 | 93.11312529 | 1.240183442 |
| Ba XI IP | 146.5212 | | | |

## Table B.23: Ba II

| Ba | Z | | a | |
|---|---|---|---|---|
| 2 | 56 | | 2 | |
| **Configuration** | **NIST (eV)** | **X** | **Equation (1)** | **Δ%** |
| 6s | 0.000000 | | | |
| 7s | 5.2513724 | 1 | 5.1031137 | 2.8232381 |
| 8s | 7.1942092 | 2 | 7.1043665 | 1.2488202 |
| 9s | 8.1437341 | 3 | 8.0898824 | 0.6612653 |
| 10s | 8.6807020 | 4 | 8.6466437 | 0.3923449 |
| 11s | 9.0143060 | 5 | 8.9915877 | 0.2520253 |
| 12s | 9.2357850 | 6 | 9.2199723 | 0.1712113 |
| 20s | 9.8020720 | 14 | 9.7998046 | 0.0231322 |
| 21s | 9.8245700 | 15 | 9.8226676 | 0.0193636 |
| 22s | 9.8434940 | 16 | 9.8418923 | 0.0162716 |
| 23s | 9.8595930 | 17 | 9.8582116 | 0.0140109 |
| 24s | 9.8733670 | 18 | 9.8721827 | 0.0119945 |
| 25s | 9.8852630 | 19 | 9.8842355 | 0.0103938 |
| 35s | 9.9487110 | 29 | 9.9483904 | 0.0032226 |
| 36s | 9.9520600 | 30 | 9.9517665 | 0.0029494 |
| 37s | 9.9551070 | 31 | 9.9548433 | 0.0026492 |
| 38s | 9.9579060 | 32 | 9.9576552 | 0.0025190 |
| 39s | 9.9604560 | 33 | 9.9602317 | 0.0022521 |
| 40s | 9.9627940 | 34 | 9.9625984 | 0.0019632 |
| 41s | 9.9649570 | 35 | 9.9647775 | 0.0018013 |
| 42s | 9.9669480 | 36 | 9.9667883 | 0.0016024 |
| 43s | 9.9687920 | 37 | 9.9686477 | 0.0014479 |
| 44s | 9.9705030 | 38 | 9.9703705 | 0.0013293 |
| 45s | 9.9721000 | 39 | 9.9719697 | 0.0013064 |
| 46s | 9.9735750 | 40 | 9.9734570 | 0.0011831 |
| 47s | 9.9749590 | 41 | 9.9748425 | 0.0011678 |
| 48s | 9.9762470 | 42 | 9.9761353 | 0.0011195 |
| 49s | 9.9774400 | 43 | 9.9773435 | 0.0009671 |
| Ba III IP | 10.003826 | | | |

## Sixth Period

### Table B.24: Au I

| Au<br>1 | Z<br>79 | | a<br>1 | |
|---|---|---|---|---|
| **Configuration** | **NIST (eV)** | **X** | **Equation (1)** | **Δ%** |
| $5d^{10}6s$ | 0.0000000 | | | |
| $5d^{10}7s$ | 6.7553081 | 1 | 6.4509271 | 4.50580 |
| $5d^{10}8s$ | 8.0270300 | 2 | 7.9087620 | 1.47337 |
| $5d^{10}9s$ | 8.5153000 | 3 | 8.4595242 | 0.65501 |
| $5d^{10}10s$ | 8.7554300 | 4 | 8.7251640 | 0.34568 |
| $5d^{10}11s$ | 8.8913800 | 5 | 8.8732489 | 0.20392 |
| $5d^{10}12s$ | 8.9759500 | 6 | 8.9641472 | 0.13149 |
| $5d^{10}13s$ | 9.0319400 | 7 | 9.0239191 | 0.08881 |
| $5d^{10}14s$ | 9.0709400 | 8 | 9.0653094 | 0.06207 |
| **Au I IP** | 9.2255540 | | | |

### Table B.25: Hg II

| Hg<br>2 | Z<br>80 | | a<br>2 | |
|---|---|---|---|---|
| **Configuration** | **NIST (eV)** | **X** | **Equation (1)** | **Δ%** |
| $5d^{10}6s$ | 0.0000000 | | | |
| $5d^{10}7s$ | 11.8670738 | 1 | 11.3101139 | 4.69332 |
| $5d^{10}8s$ | 15.0537429 | 2 | 14.7887592 | 1.76025 |
| $5d^{10}9s$ | 16.4354134 | 3 | 16.2967310 | 0.84380 |
| $5d^{10}10s$ | 17.1637129 | 4 | 17.0837974 | 0.46561 |
| $5d^{10}11s$ | 17.5948783 | 5 | 17.5457380 | 0.27929 |
| **Hg II IP** | 18.75687 | | | |

# Seventh Period

## Table B.26: Fr I

| Fr<br>1 | | Z<br>87 | | a<br>1 | |
|---|---|---|---|---|---|
| **Configuration** | | **NIST (eV)** | **X** | **Equation (1)** | **Δ%** |
| 7s | | 0.0000000 | | | |
| 8s | | 2.4474460 | 1 | 2.3712193 | 3.11454 |
| 9s | | 3.1827980 | 2 | 3.1441340 | 1.21478 |
| 10s | | 3.5100691 | 3 | 3.4889877 | 0.60060 |
| 11s | | 3.6846751 | 4 | 3.6721355 | 0.34032 |
| 12s | | 3.7888956 | 5 | 3.7808885 | 0.21133 |
| 13s | | 3.8560994 | 6 | 3.8506942 | 0.14017 |
| 14s | | 3.9019643 | 7 | 3.8981514 | 0.09772 |
| 15s | | 3.9346611 | 8 | 3.9318737 | 0.07084 |
| 16s | | 3.9587893 | 9 | 3.9566919 | 0.05298 |
| 17s | | 3.9771021 | 10 | 3.9754855 | 0.04065 |
| 18s | | 3.9913304 | 11 | 3.9900578 | 0.03188 |
| 19s | | 4.0026042 | 12 | 4.0015844 | 0.02548 |
| 20s | | 4.0116877 | 13 | 4.0108585 | 0.02067 |
| 21s | | 4.0191139 | 14 | 4.0184310 | 0.01699 |
| 22s | | 4.0252631 | 15 | 4.0246940 | 0.01414 |
| 23s | | 4.0304130 | 16 | 4.0299330 | 0.01191 |
| 24s | | 4.0347670 | 17 | 4.0343596 | 0.01010 |
| 25s | | 4.0384830 | 18 | 4.0381334 | 0.00866 |
| 26s | | 4.0416790 | 19 | 4.0413769 | 0.00748 |
| 27s | | 4.0444480 | 20 | 4.0441848 | 0.00651 |
| 28s | | 4.0468620 | 21 | 4.0466319 | 0.00569 |
| 29s | | 4.0489790 | 22 | 4.0487774 | 0.00498 |
| 30s | | 4.0508480 | 23 | 4.0506689 | 0.00442 |
| **Fr I IP** | **4.0727410** | | | | |

# 12. Appendix C - Single and Multi-Electron Results for Fine-Structure Energy Splits $E_\Delta$ (Eq. 6)

It will be shown in Appendix C that the fine-structure energy splits will be more accurate for heavier elements (on the order of 3%) with accuracy decreasing, with still acceptable accuracy, to the multi-electron He I. This is the reverse of the case for the principal lines.

All energies are in electron volts.

**Table C.1: Ge XXXII**

| $p\left(E_{\left(\frac{3}{2}\right)} - E_{\left(\frac{1}{2}\right)}\right);\ d\left(E_{\left(\frac{5}{2}\right)} - E_{\left(\frac{3}{2}\right)}\right);\ f\left(E_{\left(\frac{7}{2}\right)} - E_{\left(\frac{5}{2}\right)}\right);$<br>$I_e = 14119.430$ | | | | | |
|---|---|---|---|---|---|
| **n** | **2s** | **3s** | **4s** | **5s** | **6s** |
| **NIST** | **10576.4097** | **12550.1052** | **13238.9431** | **13556.9386** | **-** |
| **Eq. A.10** | **3506.3403** | **1554.9126** | **873.6674** | **558.7748** | **-** |
| **$E_n$ (ev)** | **10613.0897** | **12564.5174** | **13245.7626** | **13560.6552** | **-** |
| **Δ%** | **0.35%** | **0.11%** | **0.052%** | **0.027%** | |
| **S=1** | **2p** | **3p** | **4p** | **5p** | **6p** |
| **NIST** | **49.2599** | **14.6092** | **6.1562** | **3.148** | **-** |
| **Eq. B.5.** | **47.9592** | **14.1628** | **5.9650** | **3.051** | **-** |
| **Δ%** | **2.6%** | **3.1%** | **3.1%** | **3.1%** | |
| **S=3** | | **3d** | **4d** | **5d** | **6d** |
| **NIST** | | **4.7451** | **2.0042** | **1.0264** | **-** |
| **Eq. B.5.** | | **4.7209** | **1.9883** | **1.0170** | **-** |
| **Δ%** | | **0.51%** | **0.79%** | **0.92%** | |
| **S=6** | | | **4f** | **5f** | **6f** |
| **NIST** | | | **0.9958** | **0.5102** | **-** |
| **Eq. B.5.** | | | **0.9941** | **0.5085** | **-** |
| **Δ%** | | | **0.17%** | **0.33%** | |
| **S=10** | | | | **5g** | **6g** |
| **NIST** | | | | **0.3054** | **-** |
| **Eq. B.5.** | | | | **0.3051** | **-** |
| **Δ%** | | | | **0.098%** | |

## Table C.2: Ge XXXI

| $p\left(E_{(2)} - E_{(0)}\right); d\left(E_{(3)} - E_{(2)}\right)$<br>$I_e = 13557.4207$ | | | | | |
|---|---|---|---|---|---|
| **n** | **2s** | **3s** | **4s** | **5s** | **6s** |
| **NIST** | **10201.12935** | **12075.7019** | **-** | **-** | **-** |
| **Eq. A.10** | **3328.2424** | **1470.3282** | **-** | | **-** |
| **$E_n$ (ev)** | **10229.17834** | **12087.0925** | **-** | **-** | **-** |
| **Δ%** | **0.27%** | **0.094%** | | | |
| **S=1** | **2p** | **3p** | **4p** | **5p** | **6p** |
| **NIST** | **40.7251** | **12.1207** | **-** | **-** | **-** |
| **Eq. B.5.** | **42.9660** | **12.6161** | **-** | **-** | **-** |
| **Δ%** | **5.5%** | **4.1%** | | | |
| **S=3** | | **3d** | **4d** | **5d** | **6d** |
| **NIST** | | **4.0815** | **-** | **-** | **-** |
| **Eq. B.5.** | | **4.2054** | **-** | **-** | **-** |
| **Δ%** | | **3.0%** | | | |

## Table C.3: Ge XXX

| $p\left(E_{\left(\frac{3}{2}\right)} - E_{\left(\frac{1}{2}\right)}\right); d\left(E_{\left(\frac{5}{2}\right)} - E_{\left(\frac{3}{2}\right)}\right);\ f\left(E_{\left(\frac{7}{2}\right)} - E_{\left(\frac{5}{2}\right)}\right)$<br>$I_e = 3194.293$ | | | | | |
|---|---|---|---|---|---|
| **n** | **2s** | **3s** | **4s** | **5s** | **6s** |
| **NIST** | **3194.293** | **1792.19** | **-** | **-** | **-** |
| **Eq. A.10** | **-** | **1399.56** | **781.6816** | **-** | **-** |
| **$E_n$ (ev)** | **-** | **1794.73** | **2412.6114** | **-** | **-** |
| **Δ%** | | **0.14%** | | | |
| **S=1** | **2p** | **3p** | **4p** | **5p** | **6p** |
| **NIST** | **39.1402** | **11.40** | **-** | **-** | **-** |
| **Eq. B.5.** | **39.0952** | **11.34** | **-** | **-** | **-** |
| **Δ%** | **0.11%** | **0.53%** | | | |
| **S=3** | | **3d** | **4d** | **5d** | **6d** |
| **NIST** | | **3.10** | **1.3** | **-** | **-** |
| **Eq. B.5.** | | **3.78** | **1.58** | **-** | **-** |
| **Δ%** | | **21.9%** | **21.5%** | | |
| **S=6** | | | **4f** | **5f** | **6f** |
| **NIST** | | | **0.12** | **-** | **-** |
| **Eq. B.5.** | | | **0.79** | **-** | **-** |
| **Δ%** | | | **84.8%** | | |

**Table C.4: Ga XXXI**

| $\boldsymbol{p\left(E_{\left(\frac{3}{2}\right)} - E_{\left(\frac{1}{2}\right)}\right); d\left(E_{\left(\frac{5}{2}\right)} - E_{\left(\frac{3}{2}\right)}\right); f\left(E_{\left(\frac{7}{2}\right)} - E_{\left(\frac{7}{2}\right)}\right);}$<br>$\boldsymbol{I_e = 13329.489}$ | | | | | |
|---|---|---|---|---|---|
| **n** | **2s** | **3s** | **4s** | **5s** | **6s** |
| **NIST** | **9918.0286** | **11767.9837** | **10845.9417** | **12711.9130** | **-** |
| **Eq. A.10** | **3289.2236** | **1458.8372** | **717.0939** | **524.3083** | **-** |
| $\boldsymbol{E_n}$ **(ev)** | **9950.8322** | **11780.6518** | **10849.8036** | **12715.1807** | **-** |
| **Δ%** | **0.33%** | **0.11%** | **0.036%** | **0.026%** | |
| **S=1** | **2p** | **3p** | **4p** | **5p** | **6p** |
| **NIST** | **43.2913** | **12.8387** | **5.4095** | **2.7668** | **-** |
| **Eq. B.5.** | **42.2126** | **12.4634** | **5.2519** | **2.6864** | **-** |
| **Δ%** | **2.5%** | **2.9%** | **2.9%** | **2.9%** | |
| **S=3** | | **3d** | **4d** | **5d** | **6d** |
| **NIST** | | **4.17675** | **1.76395** | **0.90325** | **-** |
| **Eq. B.5.** | | **4.15615** | **1.75064** | **0.89549** | **-** |
| **Δ%** | | **0.49%** | **0.75%** | **0.86%** | |
| **S=6** | | | **4f** | **5f** | **6f** |
| **NIST** | | | **0.87679** | **0.44919** | **-** |
| **Eq. B.5.** | | | **0.87532** | **0.44774** | **-** |
| **Δ%** | | | **0.17%** | **0.32%** | |
| **S=10** | | | | **5g** | **6g** |
| **NIST** | | | | **0.26889** | **-** |
| **Eq. B.5.** | | | | **0.26865** | **-** |
| **Δ%** | | | | **0.089%** | |

## Table C.5: Ga XXX

$$p\left(E_{(2)} - E_{(0)}\right); d\left(E_{(3)} - E_{(2)}\right)$$

$$I_e = 12696.5573$$

| n | 2s | 3s | 4s | 5s | 6s |
|---|---|---|---|---|---|
| NIST | 9555.27675 | 11309.76885 | 11919.5555 | - | - |
| Eq. A.10 | 3116.94402 | 1376.9876 | 772.2311 |  | - |
| $E_n$ (ev) | 9579.61328 | 11319.56989 | 11924.3262 | - | - |
| Δ% | 0.25% | 0.087% | 0.040% |  |  |
|  |  |  |  |  |  |
| S=1 | 2p | 3p | 4p | 5p | 6p |
| NIST | 35.6095 | 10.5846 | 4.564 | - | - |
| Eq. B.5. | 37.6838 | 11.0652 | 4.647 | - | - |
| Δ% | 5.8% | 4.5% | 1.8% |  |  |
| S=3 |  | 3d | 4d | 5d | 6d |
| NIST |  | 3.5671 | 1.500 | - | - |
| Eq. B.5. |  | 3.6884 | 1.549 | - | - |
| Δ% |  | 3.4% | 3.3% |  |  |

## Table C.6: Ga XXIX

$$p\left(E_{\left(\frac{3}{2}\right)} - E_{\left(\frac{1}{2}\right)}\right); d\left(E_{\left(\frac{5}{2}\right)} - E_{\left(\frac{3}{2}\right)}\right); \ f\left(E_{\left(\frac{7}{2}\right)} - E_{\left(\frac{7}{2}\right)}\right)$$

$$I_e = 2984.426$$

| n | 2s | 3s | 4s | 5s | 6s |
|---|---|---|---|---|---|
| NIST | 2984.426 | 1675.0798 | 2252.7234 | 2518.0682 | - |
| Eq. A.10 | - | 1307.6760 | 730.3819 | 465.4699 | - |
| $E_n$ (ev) | - | 1676.7500 | 2254.0441 | 2518.9561 | - |
| Δ% |  | 0.10% | 0.059% | 0.035% |  |
| S=1 | 2p | 3p | 4p | 5p | 6p |
| NIST | 34.1403 | 10.1072 | 4.2588 | 2.1784 | - |
| Eq. B.5. | 34.1295 | 9.8990 | 4.1320 | 2.1022 | - |
| Δ% | 0.032% | 2.1% | 3.0% | 3.5% |  |
| S=3 |  | 3d | 4d | 5d | 6d |
| NIST |  | 3.1913 | 1.3468 | 0.6893 | - |
| Eq. B.5. |  | 3.3000 | 1.3773 | 0.7008 | - |
| Δ% |  | 3.4% | 2.3% | 1.7% |  |

## Table C.7: Cu XXIX

| $p\left(E_{\left(\frac{3}{2}\right)} - E_{\left(\frac{1}{2}\right)}\right); d\left(E_{\left(\frac{5}{2}\right)} - E_{\left(\frac{3}{2}\right)}\right); f\left(E_{\left(\frac{7}{2}\right)} - E_{\left(\frac{5}{2}\right)}\right);$<br>$I_e = 11567.613$ | | | | | |
|---|---|---|---|---|---|
| **n** | **2s** | **3s** | **4s** | **5s** | **6s** |
| **NIST** | 8666.8376 | 10281.9549 | 10845.9417 | 11106.4270 | - |
| **Eq. A.10** | 2876.1862 | 1275.9892 | 717.0939 | 458.6908 | - |
| $E_n$ **(ev)** | 8691.4268 | 10291.6239 | 10849.8036 | 11108.9222 | - |
| **Δ%** | 0.28% | 0.094% | 0.036% | 0.022% | |
| **S=1** | **2p** | **3p** | **4p** | **5p** | **6p** |
| **NIST** | 33.0195 | 9.797 | 4.1262 | 2.111 | - |
| **Eq. B.5.** | 32.2897 | 9.541 | 4.0198 | 2.056 | - |
| **Δ%** | 2.2% | 2.6% | 2.6% | 2.6% | |
| **S=3** | | **3d** | **4d** | **5d** | **6d** |
| **NIST** | | 3.1951 | 1.349 | 0.6912 | - |
| **Eq. B.5.** | | 3.1805 | 1.340 | 0.6855 | - |
| **Δ%** | | 0.46% | 0.67% | 0.82% | |
| **S=6** | | | **4f** | **5f** | **6f** |
| **NIST** | | | 0.6716 | 0.3437 | - |
| **Eq. B.5.** | | | 0.6700 | 0.3428 | - |
| **Δ%** | | | 0.24% | 0.26% | |
| **S=10** | | | | **5g** | **6g** |
| **NIST** | | | | 0.2058 | - |
| **Eq. B.5.** | | | | 0.2057 | - |
| **Δ%** | | | | 0.049% | |

## Table C.8: Cu XXVIII

$$p\left(E_{(2)}-E_{(0)}\right);\ d\left(E_{(3)}-E_{(2)}\right)$$

$$I_e = 11062.4312$$

| n | 2s | 3s | 4s | 5s | 6s |
|---|---|---|---|---|---|
| NIST | 8329.2801 | 9855.7205 | 10386.212 | 10630.715 | - |
| Eq. A.10 | 2715.4866 | 1199.5290 | 672.734 | 429.770 | - |
| $E_n$ (ev) | 8346.9446 | 9862.8392 | 10389.697 | 10632.661 | - |
| Δ% | 0.21% | 0.072% | 0.034% | 0.018% | |
| S=1 | 2p | 3p | 4p | 5p | 6p |
| NIST | 26.7831 | 7.961 | 3.359 | - | - |
| Eq. B.5. | 28.6002 | 8.334 | 3.527 | - | - |
| Δ% | 6.8% | 4.7% | 5.0% | | |
| S=3 | | 3d | 4d | 5d | 6d |
| NIST | | 2.691 | 1.14 | - | - |
| Eq. B.5. | | 2.736 | 1.18 | - | - |
| Δ% | | 1.7% | 3.5% | | |

## Table C.9: Cu XXVII

$$p\left(E_{\left(\frac{3}{2}\right)}-E_{\left(\frac{1}{2}\right)}\right);\ d\left(E_{\left(\frac{5}{2}\right)}-E_{\left(\frac{3}{2}\right)}\right);\ f\left(E_{\left(\frac{7}{2}\right)}-E_{\left(\frac{5}{2}\right)}\right)$$

$$I_e = 2586.954$$

| n | 2s | 3s | 4s | 5s | 6s |
|---|---|---|---|---|---|
| NIST | 2586.954 | 1452.3980 | 1952.9668 | 2182.891 | - |
| Eq. A.10 | - | 1133.520215 | 633.1108 | 403.480 | - |
| $E_n$ (ev) | - | 1453.4338 | 1953.8432 | 2183.474 | - |
| Δ% | | 0.071% | 0.045% | 0.027% | |
| S=1 | 2p | 3p | 4p | 5p | 6p |
| NIST | 25.6091 | 7.5829 | 3.1963 | 1.6339 | - |
| Eq. B.5. | 25.6441 | 7.4379 | 3.1047 | 1.5799 | - |
| Δ% | 0.14% | 1.9% | 2.9% | 3.3% | |
| S=3 | | 3d | 4d | 5d | 6d |
| NIST | | 2.3954 | 1.0119 | 0.5561 | - |
| Eq. B.5. | | 2.4793 | 1.0349 | 0.5268 | - |
| Δ% | | 3.5% | 2.3% | 5.3% | |
| S=6 | | | 4f | 5f | 6f |
| NIST | | | 0.451 | - | - |
| Eq. B.5. | | | 0.517 | - | - |
| Δ% | | | 14.6% | | |

## Table C.10: Ne X

**$p\left(E_{\left(\frac{3}{2}\right)} - E_{\left(\frac{1}{2}\right)}\right)$; $d\left(E_{\left(\frac{5}{2}\right)} - E_{\left(\frac{3}{2}\right)}\right)$; $f\left(E_{\left(\frac{7}{2}\right)} - E_{\left(\frac{5}{2}\right)}\right)$; etc.**

**$I_e = 1362.19915$**

| n | 2s | 3s | 4s | 5s | 6s |
|---|---|---|---|---|---|
| NIST | 1021.51777 | 1210.83257 | 1277.07570 | 1307.72927 | 1324.37741 |
| Eq. A.10 | 340.34596 | 151.23469 | 85.06103 | 54.43580 | 37.80113 |
| $E_n$ (ev) | 1021.85319 | 1210.96446 | 1277.13812 | 1307.76335 | 1324.39802 |
| Δ% | 0.033% | 0.011% | 0.0049% | 0.0026% | 0.0016% |
| S=1 | 2p | 3p | 4p | 5p | 6p |
| NIST | 0.45534561 | 0.13492953 | 0.05691743 | 0.02913814 | 0.01686049 |
| Eq. B.5. | 0.45323265 | 0.13425095 | 0.05662865 | 0.02899127 | 0.01677636 |
| Δ% | 0.21% | 0.50% | 0.51% | 0.50% | 0.50% |
| S=3 |  | 3d | 4d | 5d | 6d |
| NIST |  | 0.04486734 | 0.01893052 | 9.69259E-3 | 5.60904E-3 |
| Eq. B.5. |  | 0.04475029 | 0.01887621 | 9.66376E-3 | 5.59212E-3 |
| Δ% |  | 0.26% | 0.29% | 0.30% | 0.30% |
| S=6 |  |  | 4f | 5f | 6f |
| NIST |  |  | 9.4595E-3 | 4.84357E-3 | 2.80303E-3 |
| Eq. B.5. |  |  | 9.4381E-3 | 4.83188E-3 | 2.79606E-3 |
| Δ% |  |  | 0.23% | 0.24% | 0.25% |
| S=10 |  |  |  | 5g | 6g |
| NIST |  |  |  | 2.90543E-3 | 1.68145E-3 |
| Eq. B.5. |  |  |  | 2.89913E-3 | 1.67764E-3 |
| Δ% |  |  |  | 0.22% | 0.23% |
| S=15 |  |  |  |  | 6h |
| NIST |  |  |  |  | 1.12082E-3 |
| Eq. B.5. |  |  |  |  | 1.11843E-3 |
| Δ% |  |  |  |  | 0.21% |

## Table C.11: Ne IX

| $p\left(E_{(2)}-E_{(0)}\right);\ d\left(E_{(3)}-E_{(1)}\right)$<br>$I_e = 1195.80783$ | | | | | |
|---|---|---|---|---|---|
| n | 2s | 3s | 4s | 5s | 6s |
| NIST | 910.20645 | 1070.47210 | 1125.73065 | 1151.12195 | - |
| Eq. A.10 | 286.87496 | 125.78292 | 70.27727 | 44.79628 | - |
| $E_n$ (ev) | 908.93287 | 1070.02491 | 1125.53056 | 1151.01155 | - |
| Δ% | 0.14% | 0.042% | 0.018% | 0.0096% | |
| S=1 | 2p | 3p | 4p | 5p | 6p |
| NIST | 0.2294 | 0.0694 | 0.0286 | 0.0149 | - |
| Eq. B.5. | 0.3157 | 0.0916 | 0.0383 | 0.0195 | - |
| Δ% | 37.6% | 32.0% | 33.9% | 30.9% | |
| S=3 | | 3d | 4d | 5d | 6d |
| NIST | | 0.0236 | 0.0112 | - | - |
| Eq. B.5. | | 0.0306 | 0.0128 | - | - |
| Δ% | | 29.7% | 14.3% | | |

## Table C.12: Ne VIII

| $p\left(E_{\left(\frac{3}{2}\right)}-E_{\left(\frac{1}{2}\right)}\right);\ d\left(E_{\left(\frac{5}{2}\right)}-E_{\left(\frac{3}{2}\right)}\right);\ f\left(E_{\left(\frac{7}{2}\right)}-E_{\left(\frac{5}{2}\right)}\right)$<br>$I_e = 239.0970$ | | | | | |
|---|---|---|---|---|---|
| n | 2s | 3s | 4s | 5s | 6s |
| NIST | 239.0970 | 136.36848 | 182.2092 | 203.0192 | 214.1925 |
| Eq. A.10 | - | 102.94384 | 57.0044 | 36.1431 | 24.9439 |
| $E_n$ (ev) | - | 136.15316 | 182.0926 | 202.9539 | 214.1531 |
| Δ% | | 0.16% | 0.064% | 0.032% | 0.018% |
| S=1 | 2p | 3p | 4p | 5p | 6p |
| NIST | 0.20449 | 0.06053 | 0.0255 | 0.0129 | 7.5E-3 |
| Eq. B.5. | 0.21350 | 0.06032 | 0.0248 | 0.0125 | 7.2E-3 |
| Δ% | 4.4% | 0.35% | 2.7% | 3.1% | 4.0% |
| S=3 | | 3d | 4d | 5d | 6d |
| NIST | | 0.0182 | 7.7E-3 | 4.0E-3 | 2.2E-3 |
| Eq. B.5. | | 0.0201 | 8.3E-3 | 4.2E-3 | 2.4E-3 |
| Δ% | | 10.4% | 7.8% | 5.0% | 9.1% |
| S=6 | | | 4f | 5f | 6f |
| NIST | | | 3.9E-3 | - | - |
| Eq. B.5. | | | 4.1E-3 | - | - |
| Δ% | | | 5.1% | | |

## Table C.13: He II

$p\left(E_{\left(\frac{3}{2}\right)} - E_{\left(\frac{1}{2}\right)}\right)$; $d\left(E_{\left(\frac{5}{2}\right)} - E_{\left(\frac{3}{2}\right)}\right)$; $f\left(E_{\left(\frac{7}{2}\right)} - E_{\left(\frac{5}{2}\right)}\right)$; etc.

$I_e = 54.41776503$

| n | 2s | 3s | 4s | 5s | 6s |
|---|---|---|---|---|---|
| NIST | 40.813088586 | 48.3713143135 | 51.0166680830 | 52.2410774239 | 52.9061837689 |
| Eq. A.10 | 13.60506687 | 6.046789074 | 3.401344923 | 2.176870761 | 1.511720441 |
| $E_n$ (ev) | 40.81269816 | 48.37097596 | 51.01642011 | 52.24089427 | 52.9061837689 |
| Δ% | 0.00096% | 0.00070% | 0.00046% | 0.00035% | 0.00022% |
| S=1 | 2p | 3p | 4p | 5p | 6p |
| NIST | 7.26195E-4 | 2.1516979E-4 | 9.077428E-5 | 4.64762E-5 | 2.68959E-5 |
| Eq. B.5 | 7.24472E-4 | 2.1466296E-4 | 9.056200E-5 | 4.63678E-5 | 2.68335E-5 |
| Δ% | 0.24% | 0.24% | 0.23% | 0.23% | 0.22% |
| S=3 | | 3d | 4d | 5d | 6d |
| NIST | | 7.1716397E-5 | 3.02555E-5 | 1.54909E-5 | 8.9647E-6 |
| Eq. B.5 | | 7.1554170E-5 | 3.01873E-5 | 1.54557E-5 | 8.9445E-6 |
| Δ% | | 0.23% | 0.23% | 0.23% | 0.23% |
| S=6 | | | 4f | 5f | 6f |
| NIST | | | 1.51273E-5 | 7.7452E-6 | 4.4821E-6 |
| Eq. B.5 | | | 1.50936E-5 | 7.7277E-6 | 4.4723E-6 |
| Δ% | | | 0.22% | 0.23% | 0.22% |
| S=10 | | | | 5g | 6g |
| NIST | | | | 4.64709E-6 | 2.6893E-6 |
| Eq. B.5 | | | | 4.63651E-6 | 2.6834E-6 |
| Δ% | | | | 0.23% | 0.22% |
| S=15 | | | | | 6h |
| NIST | | | | | 1.79286E-6 |
| Eq. B.5 | | | | | 1.78892E-6 |
| Δ% | | | | | 0.22% |

## Table C.14: He I

$$p(E_{(0)} - E_{(2)});\ d(E_{(1)} - E_{(3)});\ f(E_{(2)} - E_{(4)});g(E_{(3)} - E_{(5)});\ h(E_{(4)} - E_{(6)})$$

$$I_e = 24.587388804$$

| n | 2s | 3s | 4s | 5s | 6s |
|---|---|---|---|---|---|
| NIST | 20.21769482 | 22.81939202 | 23.63376478 | 23.99159333 | 24.18007937 |
| Eq. A.10 | 4.473901323 | 1.807131482 | 0.970680532 | 0.604578744 | 0.412391414 |
| $E_n$ (ev) | 20.11348748 | 22.78025732 | 23.61670827 | 23.98281006 | 24.17499739 |
| Δ% | 0.52% | 0.17% | 0.072% | 0.037% | 0.021% |
| S=1 | 2p | 3p | 4p | 5p | 6p |
| NIST | 1.3196141E-4 | 3.62802E-5 | 1.47942E-5 | 7.4351E-6 | 4.25353E-6 |
| Eq. B.5 | 6.8307282E-5 | 1.75354E-5 | 6.90351E-6 | 3.3932E-6 | 1.91145E-6 |
| Δ% | 48.2% | 51.7% | 53.3% | 54.4% | 55.1% |
| S=3 | | 3d | 4d | 5d | 6d |
| NIST | | 5.79175E-6 | 2.44521E-6 | 1.252202E-6 | 7.24682E-7 |
| Eq. B.5 | | 5.84485E-6 | 2.30133E-6 | 1.130987E-6 | 6.37027E-7 |
| Δ% | | 0.92% | 5.9% | 9.7% | 12.1% |
| S=6 | | | 4f | 5f | 6f |
| NIST | | | 1.953759E-6 | 9.28482E-7 | 5.152993E-7 |
| Eq. B.5 | | | 1.150787E-6 | 5.65440E-7 | 3.184214E-7 |
| Δ% | | | 41.1% | 39.1% | 38.2% |
| S=10 | | | | 5g | 6g |
| NIST | | | | 6.558024E-7 | 3.793168E-7 |
| Eq. B.5 | | | | 3.392218E-7 | 1.909791E-7 |
| Δ% | | | | 48.3% | 49.7% |
| S=15 | | | | | 6h |
| NIST | | | | | 2.469686E-7 |
| Eq. B.5 | | | | | 1.272579E-7 |
| Δ% | | | | | 48.5% |