International Journal of Research and Review
Volume 11; Issue: 11; November 2024
Website: www.ijrrjournal.com
E-ISSN: 2349-9788; P-ISSN: 2454-2237

Research Paper

Regression Analysis for Better Understanding of Group I Elements

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DOI: https://doi.org/10.52403/ijrr.20241153

ABSTRACT

The compatibility of mathematical prediction and their agreement with the experimental data goes long way back in the history of science – most notably Physics. One of the important branches of mathematics is statistics and regression analysis is the vital element in this realm. The precise analysis and organizing of varying data have been possible due to the statistical calculations such as regression analysis. Through the intricate calculations of raw data using statistics, it has been easier for scientists to discover patterns and logical connection within the diverse range of data and information.

Purpose: One of the important factors to distinguish the unique character of an element is its ionization energy or the energy required to make the electrons free from its atomic orbit or shell. Here, in this research, I have used the concept of Bohr's atomic theory to determine the ionization energy of Hydrogen using mathematical analysis. Similarly, I have gathered the experimentally verified ionization energy data of other Group I alkali metals, and then I have used those data to establish logical connection between the elements using the mathematical concept of regression analysis. At last, I have shown how the ionization energy of Hydrogen varies greatly from the data obtained from the line of regression; Also, I have used the experimentally found regression equation to predict the ionization energy of the new hypothetical alkali metals having atomic number 119: which is yet to be experimentally verified. The main aim of this research was to show the mathematical relationship of the alkali metals and their compatibility with each other based on statistical analysis. Similarly, another purpose was to hypothetically establish the same coherent relationship between the alkali metals and unverified hypothetical element 119 using the underlying concept of statistics and mathematics.

Statistical Methods: The atomic model of the, Danish physicist, Niels Bohr is used as a base model to calculate the ionization energy of Hydrogen; however, due to the limitation of the Bohr's concept, the same method cannot be used to calculate the ionization energy of multiple electron system atoms. For this reason, experimentally verified ionization energy of alkali metals is taken as a raw data for the computational calculation of the line of regression and their corresponding equations.

Keywords: Bohr's atomic model, Regression analysis, Group I alkali metals, ionization energy (ground state level energy), Rydberg Constant, Planck Constant.

INTRODUCTION

Great Scientist Niels Bohr incorporated his scientific discovery through his explicit study of Hydrogen atom to create a foundational understanding of the subatomic particle such as electron, atomic energy that binds the electron and nucleus, and the electron orbitals where electrons revolve around the nucleus. Although, Bohr chose to study the atomic structure of a simple Hydrogen atom as compared to other complex multi electron atoms, it provided revolutionary ideas to further explore the colossal realms of the quantum mechanics. Similarly, the theory is in good agreement with the experimentally found results of ground state energy, and spectral lines produced by Hydrogen atoms. Here, we deep dive into Bohr's theory to find out the ionization energy of Hydrogen atom so that we can compare the result with the values of other Group I elements named as alkali metals.

Ionization Energy:

Ionization energy is the same ground state level energy that binds the electron in its particular orbital shells- quantum number represented by n in quantum mechanical model- with its atomic nucleus; so, to liberate the electrons completely from its orbital shells, electrons shall be provided with the same amount of energy that causes the electron to break the bondage of atomic nucleus and be a free electron inside an atom. In case of atoms with multiple electrons in its multiple orbits or shells, there accounts interelectronic repulsion and shielding effect other different effects which makes the simple mathematical analysis of atomic energy inaccurate, so more broad computational calculations are needed to determine the ionization energy in case of atoms with multiple electrons exerting repulsive force with each other.

Regression analysis:

It is a statistical calculation between two variable data that are generally correlated with each other and the mathematical analysis helps us to best predict the value of one variable when value of another variable is given using the line of regression or regression equation. Two lines of regression are calculated in which one line represents the line of regression of X (values assigned to first category) on Y (values assigned to second category) and another line represents the line of regression of Y on X. The equation of former line is used to best estimate the value of Y when the value of X variable and the equation of latter line used vice versa.

MATERIALS & METHODS

Here, in this research paper, the value of atomic number and their corresponding values of first ionization energy(second and third ionization energy are different and require different calculations and give different results) is taken as 1st and 2nd variable respectively in the regression analysis. Then, same values are used to produce the required regression equation and the consequential lines in the graphical chart. **Note:** the values of ionization energies of all the elements are taken in the unit of **eV** (electron Volt) for the calculation of regression line in this paper.

The experimentally valid data of ionization energy of alkali metals has been gathered from the valid sources which have conducted precise lab experiment on the atomic level. [Source of ionization data: NIST Atomic Spectra Database, Ionization Energies Data.] But, in case of Hydrogen the ionization energy is calculated using the simple mathematical analysis of Bohr's model. In the mathematical experiment, the atomic number of alkali elements is taken as one variable and its ground state level energy is taken as another variable. Then, both the data are used to find the lines of regression of 2nd variable on 1st variable. Moreover, the same method helps us to predict the ionization energy of the hypothetical element 119 named as Ununennium and shows its congruency with the ionization energy trend of the Group 1st alkali metals. However, in the case of Hydrogen the trend of ionization energy of alkali metals doesn't seem to be abide at all.

Approach of calculation:

All the mathematical calculation has been thoroughly performed with precise measurement, and only the important calculations and expressions are presented here in this paper to make the paper more concise in terms of volume. In essence, the calculated data are represented here through the help of graphs and charts to add more depth to the results. The discussion and outcomes are mentioned here after performing the in-depth analysis of the mathematical results obtained using the standard method of regression analysis.

STATISTICAL ANALYSIS AND RESULTS

Hydrogen being the simple one electron system of element makes it easier to apply the concept of Bohr's atomic model to yield out the ionization energy or the ground state energy of an electron bounded to the atomic nucleus. Using the postulates of Bohr's atomic model and performing the mathematical calculations on the theory, we arrive at the conclusion that the total amount of energy required by an electron inside an atom to completely liberate itself from the orbital shells is equal to the total energy that binds the electron inside the orbit along with the attraction to the nucleus containing proton and neutron.

Based on Bohr's atomic theory,
Total energy exerted on the electron in the nth orbit (number of the orbit where electron is currently located) is equal to the sum of its Kinetic and Potential energy. The kinetic energy is due to the motion of an electron.

Mathematical expression is:

Et = Ek + Ep (Where **Et** is the total energy binding the electron, **Ek** and **Ep** is the total kinetic energy and potential energy of an electron respectively.) = $\frac{me^4.Z^2}{8\mathcal{E}o^2nh} - \frac{me^4.Z^2}{4\mathcal{E}o^2n^2h^2}$

$$\textbf{Et} = -\frac{me^4.Z^2}{8\mathcal{E}o^2n^2h^2} \longrightarrow \text{Eq.(1.1)}$$

Where, m= mass of electron
e = charge of an electron
Z = atomic number of an element
$\mathcal{E}o =$ permittivity of free space between nucleus and orbit
n = principal quantum number
h = planck's constant

*Note: (-) negative sign shows that the electron is bound to the nucleus. So, energy is required to separate electron away from the influence of nucleus. The same energy is called as the required ionization energy.

In the case of Hydrogen atom, the value of Z = 1 and putting all the values of m, e, $\mathcal{E}o$, and h in the eq. (1.1) we get,

$$\textbf{Et} = -\frac{13.6}{n^2}\text{ eV} \longrightarrow \text{Eq. (1.2)}$$

(eV = electron Volt)

This is the required expression for the total energy of an electron of residing in the nth orbit of a Hydrogen atom.
Thus, when the value of n is 1 in the case of ground state level, the total energy of electron of a Hydrogen atom becomes -13.6 eV. And the required ionization energy of Hydrogen is – (Ground state level energy) i.e. 13.6 eV. [The heart of Physics (Grade XII) ISBN No: 978-9937-724-99-9].

Ionization Energy of Alkali Metals:
Unlike the case of Hydrogen atoms, the ionization energy of alkali metals such as Lithium, Sodium, Potassium, Rubidium, Caesium, and Francium cannot be calculated with the mere mathematical analysis of Bohr's atomic model. Indeed, the Bohr's atomic theory fails to calculate different forces and energies exerted on the heavy elements and thus requires a large scale of computational calculations to find the approximate value of their first ionization energy. The term first ionization energy is taken to refer to minimum amount of energy that is required to free the outermost electron in the outermost valence shell of an atom. The second ionization is the energy required to liberate the outermost electron – it acts a single charged ion- after one electron has been already liberated from its orbital shell; similarly, third ionization energy is the threshold energy required to remove the outermost electron- it acts as a doubly charged ions- after two electrons have already been liberated from their orbital shell. Here, in this statistical calculation, we

are using the first ionization energy of alkali metals to establish a coherent relationship between one another elements of this group.

Regression Calculation:

The atomic number of each alkali metal is taken as the element of the variable **X** in this calculation. Similarly, the respective value of their first ionization energy is taken as the element of the variable **Y** in this calculation.

Atomic Number of alkali metals(X)	**First Ionization Energy in unit eV (Y)**	**XY**	X^2
3	5.392	16.17	9
11	5.139	56.52	121
19	4.341	82.46	361
37	4.177	154.549	1369
55	3.894	213.95	3025
87	4.073	354.09	7569
$\sum x = 212$	$\sum y = 27.006$	$\sum xy = 877.748$	$\sum X^2 = 12454$

$\bar{X}$ (Mean of variable X) = 35.34
$\bar{Y}$ (Mean of variable Y) = 4.501

Mathematical Calculation and Results:

There are two regression coefficient $\mathbf{b_{yx}}$ known as the regression coefficient of y on x, and the other regression coefficient is $\mathbf{b_{xy}}$ known as the regression coefficient of x on y.

Step 1: we calculate the regression coefficient of y on x ($\mathbf{b_{yx}}$) using the standard formula of regression analysis.

$$\mathbf{b_{yx}} = \frac{n\sum xy - \sum x \sum y}{n\sum x^2 - (\sum x)^2}$$

On calculation the value of $\mathbf{b_{yx}}$ was found to be approximately – 0.0153.

Step 2: Similarly, in the same way we can calculate the value of regression coefficient of x on y ($\mathbf{b_{xy}}$).

$$\mathbf{b_{xy}} = \frac{n\sum xy - \sum x \sum y}{n\sum y^2 - (\sum y)^2}$$

On calculation the value of $\mathbf{b_{xy}}$ was found to be approximately – 40.72.

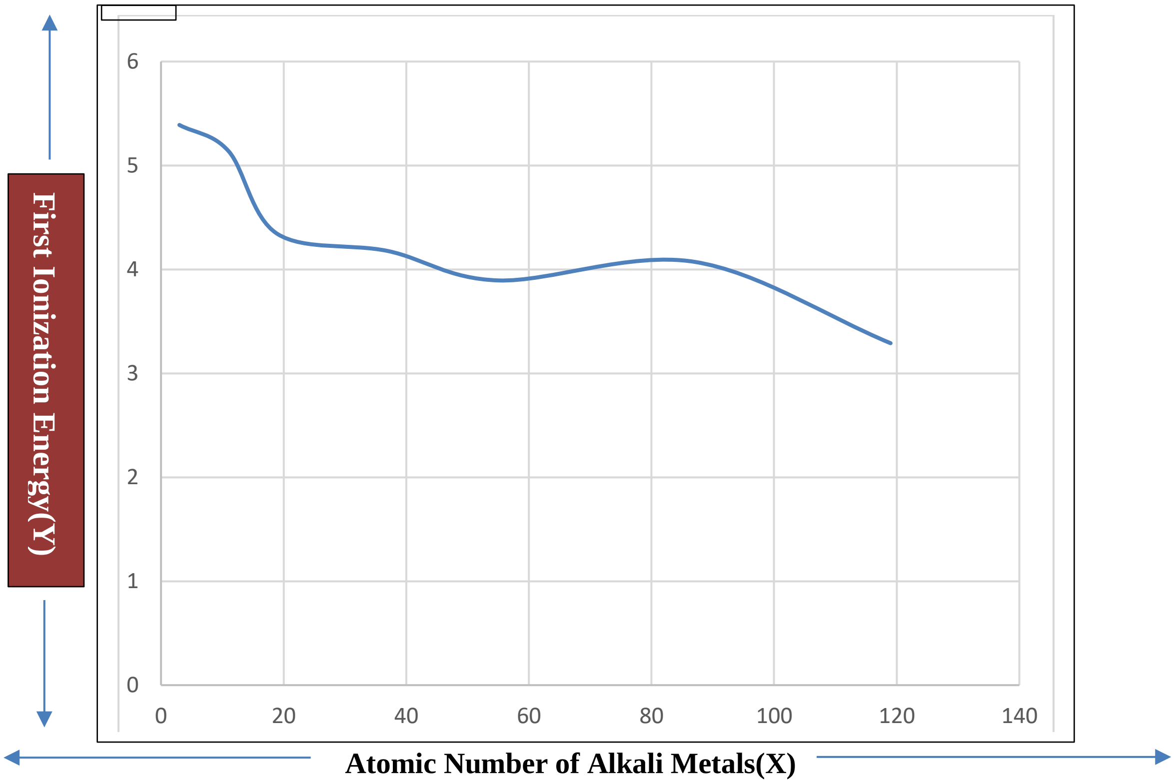
Step 3: In this step we calculate the equations of two lines of regression- line of regression of y on x and line of regression of x on y.

Regression equation of Y on X is found to be:
Y = -0.0153X + 5.0417
Regression equation of X on Y is found to be:
X = - 40.72Y + 218.62

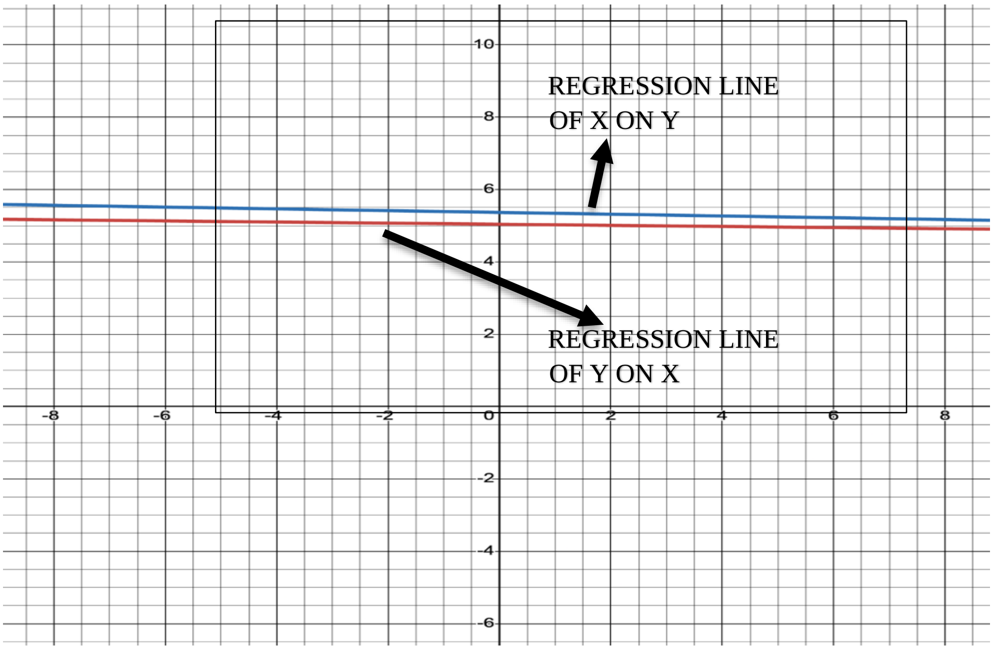
Step 4: Using these regression equations, we predict the value of Y (first ionization energy) of an hypothetical element having an atomic number (X) 119 – prophesied to show the characteristic quality of alkali metals. On calculation, the value of Y or First ionization energy was found to be approximately 3.231 which is slightly lower than the standard predicted value of approximately 4.6- 4.7 by IUPAC.

Step 5: Using the same regression equation, we find out the value of Y(ionization energy) of Hydrogen, and the output was found to be approximately 5.0264 eV. However, the experimentally verified ionization energy of Hydrogen element is 13.6 eV which is more than $2\frac{1}{2}$ half times the predicted value from the regression equation. So, the regression equation doesn’t corroborate well in case of the Hydrogen atoms.

Step 6: The experimentally proved ionization energy of all the alkali metals and the predicted value of hypothetical element- 119 is plotted in the chart to show the deflection of the line, and to better understand the compatibility of the hypothetical element with the group of other alkali metals. The first ionization energy is plotted in the Y-axis of the graphical chart, and the atomic number is plotted in the X-axis of the graphical chart.



Step 7: The above regression equations are used to create two lines of regression in the X-Y graph and the graph helps us to better understand the correlation between the two variables X and Y. By using the mathematical formula to calculate the correlation of the two variables, the value of the correlation coefficient (r) was found to be approximately -0.79 which is the high degree negative correlation and the same can observed from the graphical figure where the gap between the two line is very near and the increase in the value of one variable automatically corresponds to the decrease in value of another variable. This graph tells the best estimated value of Y variable when the value of X is known and also tells the best estimated value of X variable when the value of Y is known.



DISCUSSION

As the element- 119(referred as Ununennium) has not been yet discovered so there are chances for error of this prediction but we can assume the regression analysis is in great agreement with the overall trend showed by the ionization energy of all alkali metals. This adds another validity to the fact the element 119 may show the characteristics similar to those of alkali metals of Group I. Similarly, the standard predicted value of Ionization energy by the International Chemists association is around 4.7 for the hypothetical element, and the value is slightly higher than the value of last alkali metal Francium (Atomic Number = 87). This doesn't follow the trend that the ionization energy of the elements decreases as we go downward in the periodic table. This contradictory result may be due to the different factors that affect the electron energy of the heavy elements or the elements with high atomic number(Z) and less quantum number(n).

As we can observe the ionization energy of francium is more than that of Caesium although it has higher atomic number. It may be due to several factors such as relativistic effect on an atom. This effect occurs when the velocity of an electron so high that it causes the relative increase in its mass and thus decreasing the effective atomic radius within the atom which causes the increase in the attractive force from nucleus.

On the other hand, the shielding effect may also play out in multi electron atoms where the inner electron act as a shield to the valence electron so that it can somewhat neglect the pull of the nucleus which cause decrease in the nuclear force of attraction between the valence electron and the atomic nucleus. [Byju's Answer, Standard XII, Chemistry]. Another factor may be the interelectronic repulsion in the orbital shells with multiple electron residing in it. Considering all these complex atomic forces and factors, the standard approximate value of 4.7 predicted by international chemist committee might be more precise than the value predicted by the line of regression. However, the regression analysis can be used as a reliable method for adding another valuable agreement in the prophecy that element-119 might belong to the group of alkali metals.

Hydrogen, in the other hand seems to be completely out of the way in case of mathematical coherence of the data obtained from alkali metals. Due to the unique property of Hydrogen and its simplest atomic structure, it is difficult to correlate Hydrogen with alkali metals in terms of their compatible ionization energy. When included as a part of the alkali metals for getting the value of Ionization energy using regression analysis, Hydrogen gives the output which is not only incoherent with the experimentally verified value, but also causes the whole line of regression to be very inaccurate in terms of predicting the approximate value of ionization energy. Thus, regression analysis acts as important mathematical analysis to distinguish Hydrogen from the characteristically similar group of alkali metals.

CONCLUSION

The data generated from the regression analysis seemed to be closely in agreement with the experimental data of the ionization energy of the Group I alkali metals. The same mathematical calculation when used to predict the ionization energy of the hypothetical element referred to as Ununennium also yields a closely related value when compared to the predicted value by the International Chemist committee. But, when Hydrogen is placed in the same mathematical calculations, the results obtained are extremely contradictory to the original data obtained from lab experiment. Thus, in the basis of this calculation, it is not wrong to say that the element-119 may be more compatible with the characteristics of the alkali metals if it is ever found experimentally.

Another conclusion, that we can make from this research is that the statistical calculations such as Regression Analysis can produce nearly accurate results and predict the overall trend of the varying data with precision even in the case of complex data structures such as ionization energy of elements. In addition, the graphical representation of the data in charts made it easier for us to predict the values of unknown data and also helped us to discern the overall trend that is followed by the calculated data. In essence, this creative approach to the research has shown the new ways of understanding the logical pattern and coherence in seemingly irregular data.

Declaration by Author

Acknowledgement: I would like to express my deepest gratitude to Prof Dhruva Aryal, Head of Department of Mathematics at H.G.B.S. school, Rupandehi for his unwavering support and guidance to me during the time I endeavoured to create this research. Also, I want to thank Mr. Kedar Nath Lamsal, Head of Department of Physics for helping me to clearly understand many intricate topics of Physics.

Source of Funding: None

Conflict of Interest: No conflicts of interest declared.

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How to cite this article: Birat Neupane. Regression analysis for better understanding of group I elements. *International Journal of Research and Review*. 2024; 11(11): 531-537. DOI: *https://doi.org/10.52403/ijrr.20241153*

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