

**INVESTIGATING AND MODELING THE RELATIVE INFLUENCE OF HALOGEN TYPE
AND CHAIN LENGTH ON HALOGENOALKANE BOILING POINTS.**

1. INTRODUCTION

1.1 Background Information

Organic compounds are the foundation of biochemistry and industrial chemistry, with alkanes representing the simplest hydrocarbons, composed solely of Carbon and Hydrogen atoms connected by sigma bonds (AWD Digital). Alkanes are characterized by their low reactivity and weak intermolecular forces, particularly London Dispersion forces (LDF), due to the nonpolar nature of their molecules. However, the introduction of functional groups, such as Halogens, significantly alters the chemical and physical properties of Alkanes. This combination of Halogens bonded to Alkanes are formed when one or more hydrogen atoms in an alkane are substituted with halogen atoms, this series of compounds are called *Halogenoalkanes*, also known as alkyl halides (CH105: Chapter 7).

This substitution introduces polar carbon-halogen (C-X) bonds, as halogens are significantly more electronegative than carbon, which influence the compound's reactivity and bond strengths, influencing the physical characteristics of the compound including boiling points. The difference between electronegativity between carbon and halogens results in a polar bond with the halogen gaining a partial negative charge and the carbon a partial positive charge. This polarity introduces dipole-dipole interactions in addition to LDFs, influencing the compound's reactivity and bond strengths, which in turn impacts physical characteristics like boiling points as stated previously. The boiling point of a substance is the temperature at which its liquid phase changes into a gas. It occurs when the vapour pressure of the liquid equals the external atmospheric pressure, and essentially at the boiling point the molecules have enough energy to overcome the intermolecular forces holding them together in the liquid state. For individual atoms, the boiling point is related to the energy required to overcome intermolecular attractions (An Introduction to Halogenoalkanes).

The boiling points of pure halogens exhibit predictable periodic trends across group 17. Halogen atoms include Fluorine, Chlorine, Bromine and Iodine, which are all group 17 atoms in the periodic table. As atomic radius increases and electron affinity decreases down the group, the electron cloud polarization becomes more pronounced, thus enhancing the strength of LDFs. Consequently, the boiling points of halogens follow this periodic trend by increasing in atomic radius down the group from Fluorine to Iodine, as the number of protons increase as suggested by the atomic number, and as electron affinity decreases down the group due to greater shielding that lowers the electrostatic attraction of the added electron to the protons in the nucleus. This trend is also influenced by decreasing EN of halogens down the group, reducing the strength of Dipole-Dipole interactions in molecular compounds (LibreTexts). This relationship between Halogens and their respective boiling points are shown below:

Table 1: Halogen (diatomic) Boiling Points

Halogen	Boiling Point (°C)
F	-188.1
Cl	-34.6
Br	58.8
I	184.3

(Values Taken from *ChemSpider*)

As we can see the boiling points increase from Fluorine → Chlorine → Bromine → Iodine as per the periodic table trend. This brought me to question whether these trends of boiling points within Halogens will remain

constant within the boiling point trends of Halogenoalkanes, as the only differences in halogenoalkanes will be the Halogen type bounded to the alkyl group (methyl, ethyl...). Thus leading this investigation to examine whether halogen-based boiling point trends persist in halogenoalkanes and evaluates the relative influence of halogen type versus carbon chain length on boiling points.

1.2 Research Question, Hypothesis and Variables

Research Question: *How do halogen type and carbon chain length influence the boiling points of halogenoalkanes?*

Three hypothesis guide this study:

- 1) **Factor 1: Halogen Type Hypothesis** → Boiling points of halogenoalkanes will increase with the same periodic table trend correlation seen in halogens. Thus Fluoroalkanes < Chloroalkanes < Bromoalkanes < Iodoalkanes in terms of boiling points.
- 2) **Factor 2: Chain Length** → As chain length increases, boiling points will also increase due to strong LDFs as there are more bonds, thereby taking more energy to break for vaporization.
- 3) **Dominance hypothesis:** The Halogen Type will exert a more significant influence than chain length on the physical properties of the compound because halogens introduce varying levels of electronegativity and polarizability. These differences lead to stronger dipole-dipole interactions and London dispersion forces, especially with larger halogens. While chain length does contribute to intermolecular forces through increased Van Der Waals interactions, the pronounced effect of halogen substitution on molecular polarity and bonding will dominate the overall influence.

Independent Variables: Halogen Type, Carbon Chain Length

Dependent Variable: Boiling Points (°C)

Hence, this investigation aims to not only analyze the trends and relationships between these factors and boiling points but also to create a mathematical model that can accurately predict boiling points of halogenoalkanes.

2. METHODOLOGY

The experimental and predicted boiling point data for various halogenoalkanes were gathered from reputable sources, such as the CRC Handbook and ChemSpider. These databases provided both experimental values and predicted values for the boiling points of halogenoalkanes, allowing for comparison and validation of the experimental data. The experimental values were analyzed to assess the accuracy and consistency of the data in section 3.

The main factors for investigation were the halogen type and the chain length of the halogenoalkanes. First, the relationship between halogen type and boiling points was examined to determine if specific halogens have a greater influence on the boiling points of halogenoalkanes. Similarly, the effect of chain length on the boiling points was analyzed to identify any clear trends regarding longer or shorter carbon chains and their impact on boiling points.

A linear multivariable regression model was constructed to represent the relationship between the two independent variables (halogen type and chain length) and the dependent variable (boiling point). This model aimed to predict boiling points based on variations in halogen type and chain length. The regression analysis enabled a deeper understanding of how these factors interact and their relative contributions to boiling points, to answer the question of which factor influenced boiling point to a greater extent.

All calculations, graphing, and data analysis were conducted using Google Sheets, a reliable and widely used platform for performing such analyses. Google Sheets facilitated the creation of graphs to visually represent trends, the calculation of relative errors, and the development of the regression model.

3. RAW DATA COLLECTION

Table 2: RAW DATA VALUES COLLECTED WITH RELATIVE ERROR

Compound	Compound Formula	Halogen	Chain Length (Carbon Count)	Predicted Values: ACD/labs (± 3.0 °C)	Experimental Values: CRC (°C)	Relative Error between ACD/Labs and CRC (%) (rounded to 3 sig. figs.)	Experimental Values: OU Chemical Safety Data (°C)
Methyl Fluoride	CH ₃ F	Fluorine	1	-78.2	-78.4	-0.255	-78.5
Methyl Chloride	CH ₃ Cl	Chlorine	1	-24.5	-24.09	-1.70	-24.2
Methyl Bromide	CH ₃ Br	Bromine	1	3.8	3.5	8.57	3.6
Methyl Iodide	CH ₃ I	Iodine	1	40.3	42.43	5.02	42
Ethyl Fluoride	C ₂ H ₅ F	Fluorine	2	-36.5	-37.7	-3.18	Not available
Ethyl Chloride	C ₂ H ₅ Cl	Chlorine	2	12.7	12.3	3.25	12.3
Ethyl Bromide	C ₂ H ₅ Br	Bromine	2	39.2	38.5	1.82	38
Ethyl Iodide	C ₂ H ₅ I	Iodine	2	72.8	72.3	0.692	71
Propyl Fluoride	C ₃ H ₇ F	Fluorine	3	-0.4	-2.5	-84.0	Not available
Propyl Chloride	C ₃ H ₇ Cl	Chlorine	3	46.8	46.5	0.645	46
Propyl Bromide	C ₃ H ₇ Br	Bromine	3	71.7	71.1	0.844	Not available
Propyl Iodide	C ₃ H ₇ I	Iodine	3	102.9	102.5	0.390	101.5
Butyl Fluoride	C ₄ H ₉ F	Fluorine	4	32.8	32.5	0.923	Not available
Butyl Chloride	C ₄ H ₉ Cl	Chlorine	4	78.2	78.4	0.255	79
Butyl Bromide	C ₄ H ₉ Br	Bromine	4	101.6	101.6	0	Not available
Butyl Iodide	C ₄ H ₉ I	Iodine	4	130.9	130.5	0.307	130
Pentyl Fluoride	C ₅ H ₁₁ F	Fluorine	5	63.4	62.8	0.955	Not available
Pentyl Chloride	C ₅ H ₁₁ Cl	Chlorine	5	107.2	108.4	1.11	Not available
Pentyl Bromide	C ₅ H ₁₁ Br	Bromine	5	129.3	129.8	0.385	Not available
Pentyl Iodide	C ₅ H ₁₁ I	Iodine	5	156.9	157	0.064	Not available
Hexyl Fluoride	C ₆ H ₁₃ F	Fluorine	6	91.6	91.5	0.109	Not available
Hexyl Chloride	C ₆ H ₁₃ Cl	Chlorine	6	133.9	135.1	0.888	133

Hexyl Bromide	C ₆ H ₁₃ Br	Bromine	6	154.9	155.3	0.258	Not available
Hexyl Iodide	C ₆ H ₁₃ I	Iodine	6	181.2	181.3	0.055	Not available

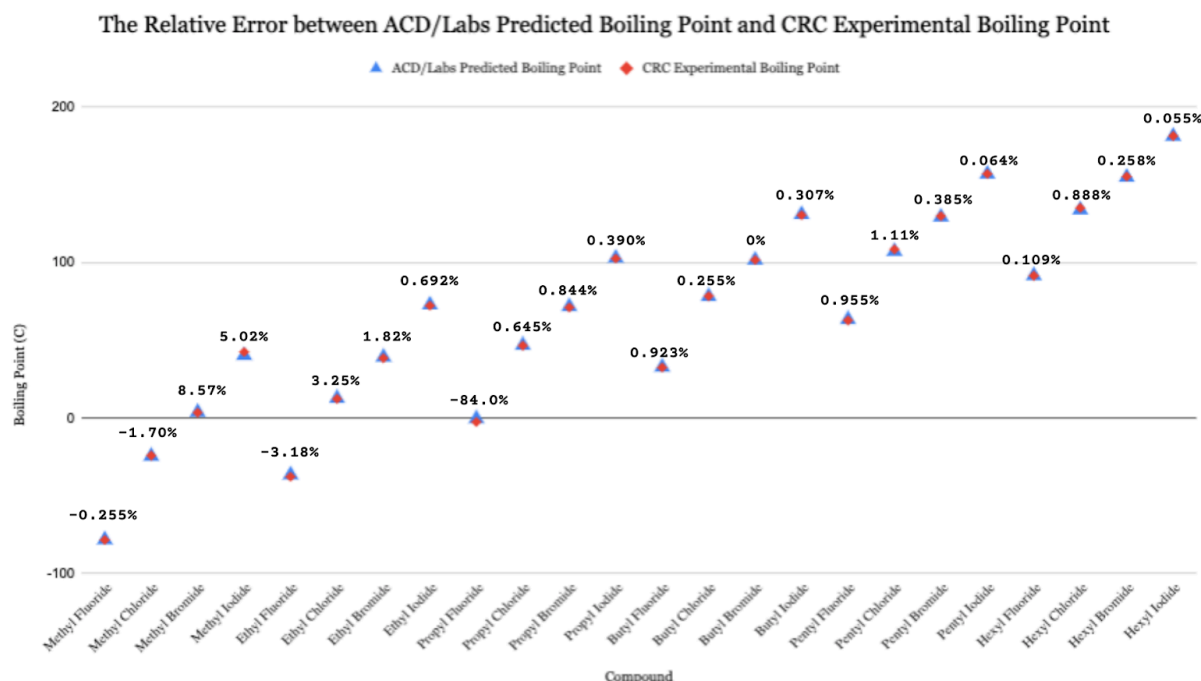
Initially, three sources of boiling point data were considered: ACD/Labs (predicted values), the CRC Handbook (experimental values), and the OU Chemical Safety Data (experimental values). However, since the OU dataset lacked data of boiling points for many compounds (as seen in Table 1 with red highlights), this dataset was ultimately excluded from the analysis. Using this data would have led to inconsistencies in comparison and ultimately seemed much more efficient to simply use the complete and reliable values.

The validity and reliability of the data between the two databases (CRC Handbook, and ACD/Labs) was tested by finding the relative error between the boiling point data values using the following formula:

$$\text{Relative Error} = \left(\frac{|\text{Experimental} - \text{Predicted}|}{\text{Experimental}} \right) \times 100$$

All relative error values were computed by Google Spreadsheets and recorded in **Table 2** and visually represented within **Figure 1**.

Figure 1: Graph comparing the boiling points from ACD/Labs Predicted, and CRC Handbook's Experimental values.



The relative error for most compounds is close to zero, indicating that both the experimental and ACD/Labs values are reliable. However, experimental values are generally preferred for maintaining realistic values and ensuring greater accuracy. Although one data point for ethyl iodide shows a significant relative error, resulting in a noticeable drop in the relative error line, this anomaly can be disregarded. All values remain within the uncertainty range of ± 3 provided by the

ACD/Labs dataset, encompassing the experimental data from the CRC Handbook. Thus for the purpose of this study, the experimental boiling point values from CRC handbook will be used.

4. ANALYSIS

4.1 Factor 1: The Effect of Halogen Types on Boiling Points

Raw Data shown from *Table 2* was graphed:

Figure 2: Graph showing the relationship between halogen types and boiling points

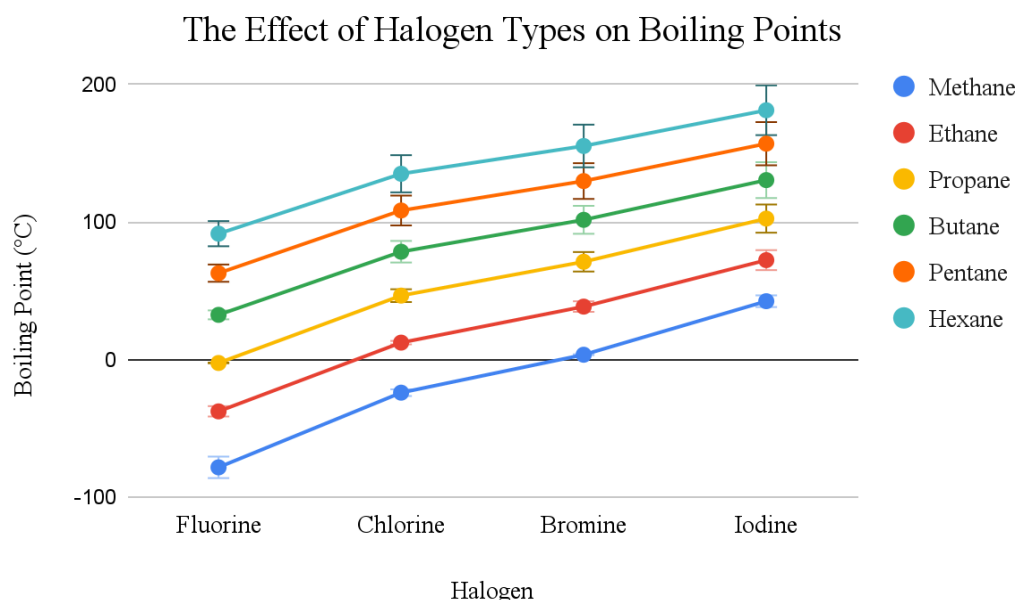


Figure 2 demonstrates a clear correlation between halogen type and boiling point, consistent with the predicted periodic trends of Group 17 elements. As the halogen changes from Fluorine to Iodine, the boiling point of the halogenoalkanes increases, as shown by the upward positive trend of the lines. This trend is evident across all chain lengths, supporting the hypothesis that Iodoalkanes will have the highest boiling points, followed by Bromoalkanes, Chloroalkanes, and Fluoroalkanes. The larger atomic radius and increased polarizability of Iodine contribute to stronger London Dispersion Forces, leading to higher boiling points.

Additionally, the introduction of halogens induces a polar carbon-halogen (C-X) bond, generating dipole-dipole interactions. While Fluoroalkanes possess the most polar bonds due to their high Electronegativity value that greatly differs from Carbon, their smaller electron cloud reduces LDF strength, resulting in lower boiling points. In contrast, Iodoalkanes exhibit less polar C-I bonds, but their significantly larger electron cloud amplifies LDF strength, dominating the overall intermolecular forces.

Thus the trend observed in the graph supports the Halogen Type hypothesis, validating the assumption that the boiling points follow the same periodic trend as the halogens themselves. Additionally, now that the trend has been confirmed to be true, we can quantify this relationship by finding the linear regression between halogen type and boiling point to work towards creating a final mathematical model to predict boiling points accurately.

To find linear regression, with categorical data such as Halogen Types, each Halogen must be given a value that is proportionate to the incremental increase in boiling points between each halogen. These values are called “dummy values” which can be determined by normalizing the mean boiling points of each halogen group onto a 0-100 scale.

The following steps are used to find the dummy values:

- 1) Calculating Mean boiling points per Halogen Type

$$Average = \frac{\Sigma Boiling Points}{Number of Boiling Points}$$

(Average calculations done by google sheets)

- 2) Determine Max and Min Values in Dataset (Indicated by **Red** values in **Table 3**)

Max: 114.3, Min: 11.4

- 3) Normalizing the Ratios

Formula:

$$Normalized Value = \frac{(Mean Value - min)}{(max - min)} \times 100$$

Fluorine Normalized Value:

$$Normalized Value = \frac{(11.4 - 11.4)}{(114.3 - 11.4)} \times 100 = 0$$

Chlorine Normalized Value:

$$Normalized Value = \frac{(59.4 - 11.4)}{(114.3 - 11.4)} \times 100 = 46.6$$

Bromine Normalized Value:

$$Normalized Value = \frac{(83.3 - 11.4)}{(114.3 - 11.4)} \times 100 = 69.9$$

Iodine Normalized Value:

$$Normalized Value = \frac{(114.3 - 11.4)}{(114.3 - 11.4)} \times 100 = 100$$

All calculated values are listed in **Table 3**

Table 3: Factor 1 - Average Boiling Points and Normalized Value per Halogen Type

Halogen Type	Average (Mean) Boiling Point (Rounded to 1 decimal place)	Normalized Value
Fluorine	11.4	0
Chlorine	59.4	46.6
Bromine	83.3	69.9
Iodine	114.3	100

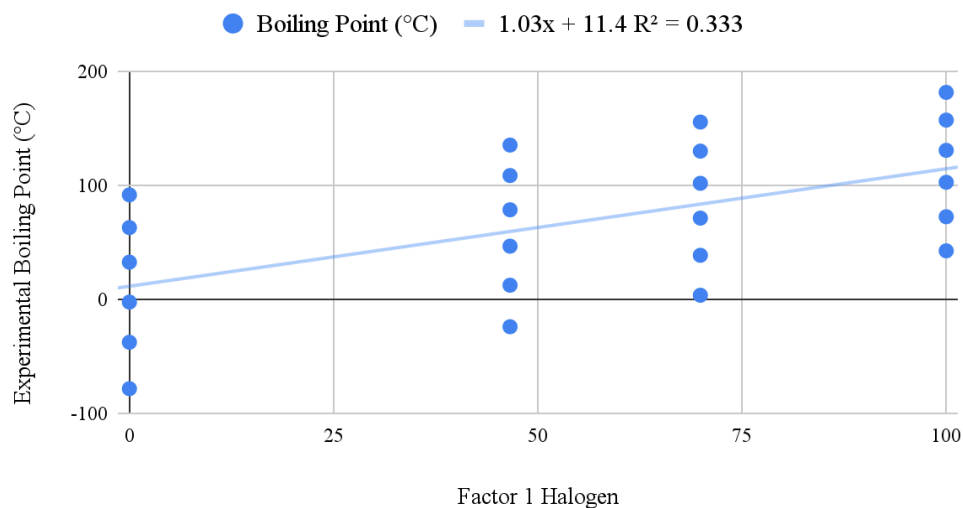
Using the following Data in **Table 4**, **Figure 3** was generated using Google Sheets to produce a regression line examining the relationship between boiling point and halogen type, to find a correlation coefficient that can be used to create a model later on using multivariable regression.

Table 4: Boiling Point Dataset with Dummy Values Representing Halogen Types to Graph.

Halogen	Halogen Value	Experimental Boiling Point (°C)
Fluorine	0	-78.4
Chlorine	46.6	-24.09
Bromine	69.9	3.5
Iodine	100	42.43
Fluorine	0	-37.7
Chlorine	46.6	12.3
Bromine	69.9	38.5
Iodine	100	72.3
Fluorine	0	-2.5
Chlorine	46.6	46.5
Bromine	69.9	71.1
Iodine	100	102.5
Fluorine	0	32.5
Chlorine	46.6	78.4
Bromine	69.9	101.6
Iodine	100	130.5
Fluorine	0	62.8
Chlorine	46.6	108.4
Bromine	69.9	129.8
Iodine	100	157
Fluorine	0	91.5
Chlorine	46.6	135.1
Bromine	69.9	155.3
Iodine	100	181.3

Figure 3: Graph with the relationship between Halogen Types and Boiling Points with Regression Line and Coefficient of Determination.

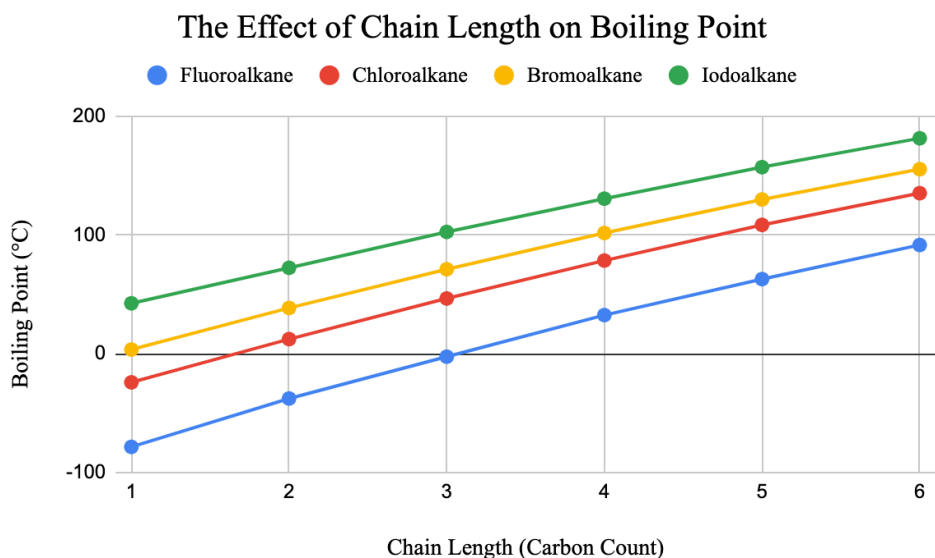
Effects of Halogen Type (Factor 1) on Boiling Point



The regression line yielded a slope of 1.03, indicating that for every unit increase in the dummy variable representing the halogen type, the boiling point increases by an average of 1.03°C. This trend supports the hypothesis that heavier halogens with larger atomic radii and stronger intermolecular forces lead to higher boiling points. The R^2 value of 0.333 suggests that halogen type accounts for 33.3% of the variance in boiling points. While this confirms a clear correlation, it also highlights the influence of additional factors, which could possibly be Chain length which will be investigated in Part 4.2. This low R^2 value indicates that halogen type alone is insufficient to predict boiling points accurately, demonstrating the need for further analysis using multivariable regression. This result aligns with the expectation that both polarizability and molecular structure contribute significantly to the boiling point variations of halogenoalkanes. The coefficient derived from this regression (1.03) will serve as a key parameter in the final predictive model, providing a baseline for understanding the influence of halogen type and other variables on boiling points of Halogenoalkanes.

4.2 The Effect of Chain Length on Boiling Points

Figure 4: Graph showing the relationship between Chain Length by Carbon Count increase and boiling points



This graph reveals a consistent positive correlation between carbon chain length and boiling points across all halogen series. As the chain length increases, the surface area and thus the electron cloud size grows, leading to stronger London Dispersion Forces. This results in higher boiling points due to the increased energy required to overcome these intermolecular forces. While all halogenoalkanes exhibit linear relationship, Iodoalkanes consistently demonstrate the highest boiling points, followed by Bromoalkanes, Chloroalkanes, and Fluoroalkanes, and this trend has been explained in part 4.1 of the analysis.

The observed relationship supports the chain length hypothesis, which predicts increasing boiling points with longer carbon chains. The proportional increase in boiling point suggests that LDF's are a dominant factor, particularly for larger molecules, more so than other intermolecular forces like dipole-dipole forces

Hence, now that the relationship between chain length and boiling point hypothesized has been confirmed to be true, we can quantify this relationship by finding the linear regression between chain length and boiling point to work towards creating a final mathematical model to predict boiling points accurately.

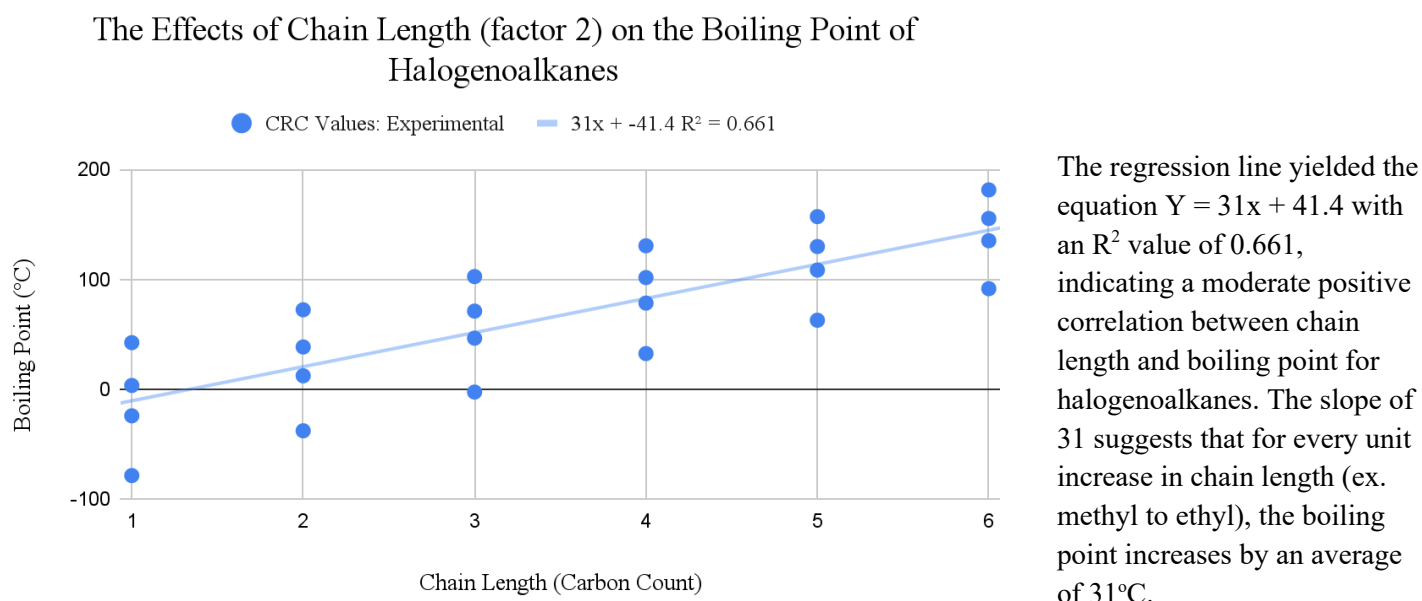
To find linear regression, the raw data shown in **Table 5** has been graphed by Google Sheets and linear regression line was generated by the platform as well.

Table 5: Data from Raw data Table used to Graph Correlation between Chain Length and Boiling Point.

Compound	Chain Length (Carbon Count)	Boiling Points
Methyl Fluoride	1	-78.4
Methyl Chloride	1	-24.09
Methyl Bromide	1	3.5
Methyl Iodide	1	42.43
Ethyl Fluoride	2	-37.7
Ethyl Chloride	2	12.3
Ethyl Bromide	2	38.5
Ethyl Iodide	2	72.3
Propyl Fluoride	3	-2.5
Propyl Chloride	3	46.5
Propyl Bromide	3	71.1
Propyl Iodide	3	102.5
Butyl Fluoride	4	32.5
Butyl Chloride	4	78.4
Butyl Bromide	4	101.6
Butyl Iodide	4	130.5

Pentyl Fluoride	5	62.8
Pentyl Chloride	5	108.4
Pentyl Bromide	5	129.8
Pentyl Iodide	5	157
Hexyl Fluoride	6	91.5
Hexyl Chloride	6	135.1
Hexyl Bromide	6	155.3
Hexyl Iodide	6	181.3

Figure 5: Graph showing the relationship between Chain Length and Boiling Point of Halogenoalkanes with a computed regression line.



This trend aligns with the expectation that longer carbon chains in halogenoalkanes generally lead to higher boiling due to increased Van der Waals forces and a larger surface area for molecular interactions. The R^2 value of 0.661 suggests that chain length accounts for 66.1% of the variance in the boiling points of halogenoalkanes. This indicates a fairly strong relationship between chain length and boiling point, though it also highlights the influence of other factors like Halogen Type that we previously investigated. Hence, the remaining 33.9% of the variance could be attributed to additional factors, emphasizing the need for a more comprehensive model that includes multiple variables.

Overall, while the regression supports the hypothesis that longer chain lengths result in higher boiling points, the moderately high R^2 value suggests that the effects of chain length is significant but not the sole factor influencing boiling point variations in halogenoalkanes. Further analysis using multivariable regression could provide a more accurate predictive model that accounts for both variables explored.

4.3 Multivariable Regression Model

Variables set for the model:

Dependent Variable (y): Boiling Point (°C)

Independent Variables (x₁, x₂):

x₁ = Chain Length (carbon count)

x₂ = Halogen Type

(Categorical variable, assigned proportional dummy values: Fluorine = 0, Chlorine = 46.6, Bromine = 69.9, Iodine = 100)

Multivariable Regression Model General Formula:

$$y = a + b_1x_1 + b_2x_2$$

Where:

y = Boiling Point (°C)

a = y-intercept

B₁ = Coefficient for relationship found with factor 1 Halogen Type and Boiling Point

B₂ = Coefficient for relationship found with factor 2 Chain Length and Boiling Point

From Parts 4.1 and 4.2 Analysis, the regression lines found are:

- **Halogen Type Regression:**

$$y = 1.03x_1 - 11.4$$

- This suggests a slope of **1.03** for halogen type

- **Chain Length Regression:**

$$y = 31x_2 - 41.1$$

- This suggests a slope of **31** for chain length

Data was analyzed on google sheets using LINEST function to produce the multivariable regression line below from the values in **Table 6** which were found from google sheets computing.

Multivariable Regression Model:

$$y = -97.16 + 1.03x_1 + 31.01x_2$$

Table 6: LINEST Function on Google Sheets used to compute the following Terms for Multivariable Regression Model

Halogen Type (b1)	31.01
Chain Length (b2)	1.03
Intercept (a)	-97.16

The coefficient of determination value was 0.995 computed by GoogleSheets for this multivariable regression model, which means that this model explains 99.5% of the variance in boiling points, which indicates a very strong fit for these factors. Also as seen from **Figure 3** and **Figure 5** from the investigation, the coefficient of determination value was 0.333 for Factor 1, and 0.661 for Factor 2, thereby confirming that these two factors do significantly influence boiling points of halogenoalkanes, but more specifically, Chain Length (factor 2) can account for majority of the variance in boiling point. This indicates that factors related to chain length, such as increased surface area and stronger London dispersion forces, have a more substantial effect on boiling points than the dipole-dipole interactions introduced by the halogen atoms. Consequently, the dominance hypothesis is rejected, as the data shows that chain length plays a more significant role in influencing the boiling points of halogenoalkanes than the type of halogen present in the molecule. This finding suggests that, while halogen type does influence boiling points, it is chain length that is the more dominant factor in determining the physical properties of these compounds.

4.4 Prediction Testing

Since the R^2 value for the multivariable regression model was 99.5% considered to be a very significant value showing that the model accounts for most variance in boiling point, we can use this model to predict boiling points, and this will confirm whether the model constructed fits this correlation.

To test, we will use the model to predict the boiling point of the compounds in the original dataset and compare these values to the experimental values used to test for accuracy of the model.

$$y = -97.16 + 1.03x_1 + 31.01x_2$$

Ex. Calculation by substitution for Methyl Fluoride

$$y = -97.16 + 1.03(0) + 31.01(1)$$

$$y = -66.15$$

(Values shown in Column 4 in Table 7)

Percent Error will be calculated using this formula:

$$\text{Percent Error} = \left| \frac{\text{Actual Value} - \text{Predicted Value}}{\text{Actual Value}} \right| \times 100$$

Ex. Calculation for Methyl Fluoride

$$\text{Percent Error} = \left| \frac{-78.4 - (-66.15)}{-78.4} \right| \times 100$$

$$\text{Percent Error} = 15.625\%$$

(Values shown in Column 6 in **Table 7**)

Table 7: Raw Data along with Predicted values from Regression Model and Percent Error of the model.

Compound	Halogen Type (#)	Chain Length (Carbon Count)	Boiling Point (°C) (Predicted by Model)	Experimental Boiling Point (°C)	Percent Error (%)
Methyl Fluoride	0	1	-66.15	-78.4	15.625
Methyl Chloride	46.6	1	-18.152	-24.09	24.64923205
Methyl Bromide	69.9	1	5.847	3.5	67.05714286
Methyl Iodide	100	1	36.85	42.43	13.15107235
Ethyl Fluoride	0	2	-35.14	-37.7	6.790450928
Ethyl Chloride	46.6	2	12.858	12.3	4.536585366
Ethyl Bromide	69.9	2	36.857	38.5	4.267532468
Ethyl Iodide	100	2	67.86	72.3	6.141078838
Propyl Fluoride	0	3	-4.13	-2.5	65.2
Propyl Chloride	46.6	3	43.868	46.5	5.660215054
Propyl Bromide	69.9	3	67.867	71.1	4.547116737
Propyl Iodide	100	3	98.87	102.5	3.541463415
Butyl Fluoride	0	4	26.88	32.5	17.29230769
Butyl Chloride	46.6	4	74.878	78.4	4.492346939
Butyl Bromide	69.9	4	98.877	101.6	2.68011811
Butyl Iodide	100	4	129.88	130.5	0.4750957854
Pentyl Fluoride	0	5	57.89	62.8	7.818471338
Pentyl Chloride	46.6	5	105.888	108.4	2.317343173
Pentyl Bromide	69.9	5	129.887	129.8	0.06702619414
Pentyl Iodide	100	5	160.89	157	2.477707006
Hexyl Fluoride	0	6	88.9	91.5	2.841530055
Hexyl Chloride	46.6	6	136.898	135.1	1.330866025
Hexyl Bromide	69.9	6	160.897	155.3	3.603992273
Hexyl Iodide	100	6	191.9	181.3	5.84666299

Therefore, the percent accuracy can be calculated in the following manner:

Step 1:

$$\begin{aligned} \text{Average Percent Error} &= \frac{\Sigma \text{Percent Errors}}{\text{Number of Data Points}} \\ \text{Average Percent Error} &= \frac{272.4103576}{24} \\ \text{Average Percent Error} &\approx 11.35\% \end{aligned}$$

Step 2:

$$\begin{aligned} \text{Percent Accuracy} &= 100 - \text{Average Percent Error} \\ \text{Percent Accuracy} &= 100 - 11.35 \\ \text{Percent Accuracy} &= 88.65\% \end{aligned}$$

Therefore, the Multivariable Regression Model used to predict the boiling points of halogenoalkanes based on chain length and halogen type demonstrated an accuracy of **88.65%**.

5. Conclusion

This study aimed to investigate how halogen type and carbon chain length influence the boiling points of halogenoalkanes. The analysis confirmed that both factors significantly affect boiling points, with chain length having a stronger influence in the increase of boiling points. While the halogen type and chain length hypotheses were supported through sections 4.1 and 4.2 of the analysis, as both factors individually led to an increase in boiling points, the effect of chain length was more pronounced. The multivariable model, which demonstrated an 88.65% accuracy in predicting boiling points, indicated a strong correlation between chain length, halogen type, and boiling point. This accuracy supports the conclusion that chain length plays the dominant role in determining boiling points, primarily due to the enhancement of London dispersion forces (LDFs) associated with increased surface area, thereby rejecting the initial dominance hypothesis.

These findings align with established scientific principles, which state that LDFs are responsible for the general trend toward higher boiling points with increased molecular mass and surface area, as observed in homologous series like alkanes (11.2 Intermolecular forces). Furthermore, having only one halogen attached to the carbon chain does not drastically increase the boiling point because the halogen bond introduces only a small change in the overall intermolecular forces. While halogens increase the boiling point by introducing dipole-dipole interactions due to their electronegativity, the effect is limited since only one bond is involved. This minor change in the intermolecular forces does not significantly outweigh the stronger influence of LDFs, which result from the larger molecular size and greater surface area of the carbon chain.

In conclusion, this study demonstrated that chain length is the primary determinant of boiling points in halogenoalkanes, with halogen type serving as a secondary factor. The results are consistent with established scientific principles, and the mathematical model provides a practical tool for predicting boiling points within the investigated scope.

6. Evaluation

In evaluating the accuracy of the model used to predict the boiling points of halogenoalkanes, it is important to address the factors that influence the observed deviations. While the model considers chain length and halogen type, it overlooks other key molecular properties and confounding variables such as the strength of London dispersion forces, polarizability, dipole-dipole interactions, and surface area. These factors contribute to the variations observed in boiling points, as

demonstrated by molecules like fluoromethane and chlorobutane, which experience stronger intermolecular forces due to their size and polarity.

Limitation	Relevance	Modification
The model does not account for variations in London dispersion forces and dipole-dipole interactions, which can significantly affect boiling points.	The strength of molecular interactions like London dispersion forces and dipole-dipole interactions directly influence boiling points, particularly in polar molecules.	Incorporate molecular size and polarizability effects to better account for intermolecular forces.
The linear relationship between chain length and halogen type oversimplifies the effect of branching and molecular structure on boiling points.	The branching of molecules affects surface area and intermolecular forces, influencing boiling point.	Use non-linear regression models to account for the complexity of molecular structure, including branching effects.
The model is based on a small dataset (24 values), limiting its reliability and generalizability to a broader range of halogenoalkanes.	A small dataset reduces the accuracy and generalizability of the predictions, making the model less reliable for a larger scope.	Increase the dataset size to include a variety of molecular structures, including branched halogenoalkanes, and longer carbon chains for better generalizability.
The linear regression model may not capture nonlinear relationships between variables, leading to inaccuracies.	Many molecular interactions exhibit non-linear relationships, especially as molecular size and complexity increase.	Implement non-linear regression techniques, such as polynomial or quadratic regression, to capture these complex relationships more effectively.
Some of the data is rounded, which can lead to small inaccuracies in the predictions	Rounding can lead to slight errors in boiling point calculations, especially when dealing with precise molecular properties.	Use more precise data to improve the accuracy of the predictions and reduce errors due to rounding, and take uncertainty values into consideration.

Works Cited

“An Introduction to Halogenoalkanes (Haloalkanes)”,

www.chemguide.co.uk/organicprops/haloalkanes/background.html. Accessed 21 Mar. 2025.

“Boiling.” *Chemistry LibreTexts*, Libretexts, 2023,

[chem.libretexts.org/Bookshelves/Physical_and_Theoretical_Chemistry_Textbook_Maps/Supplemental_Modules_\(Physical_and_Theoretical_Chemistry\)/Physical_Properties_of_Matter/States_of_Matter/Phase_Transitions/Boiling](http://chem.libretexts.org/Bookshelves/Physical_and_Theoretical_Chemistry_Textbook_Maps/Supplemental_Modules_(Physical_and_Theoretical_Chemistry)/Physical_Properties_of_Matter/States_of_Matter/Phase_Transitions/Boiling). Accessed 21 Mar. 2025.

“ChemSpider: Search and Share Chemistry - Homepage.” *ChemSpider Search and Share Chemistry*,

www.chemspider.com/. Accessed 21 Mar. 2025.

“CH105: Chapter 7 - Alkanes and Halogenated Hydrocarbons.” *Chemistry*,

wou.edu/chemistry/courses/online-chemistry-textbooks/ch105-consumer-chemistry/ch105-chapter-7/. Accessed 21 Mar. 2025.

11.2: Intermolecular Forces.” *Chemistry LibreTexts*, Libretexts, 7 July 2023,

[chem.libretexts.org/Bookshelves/General_Chemistry/Map%3A_Chemistry_-_The_Central_Science_\(Brown_et_al.\)/11%3A_Liquids_and_Intermolecular_Forces/11.02%3A_Intermolecular_Forces](http://chem.libretexts.org/Bookshelves/General_Chemistry/Map%3A_Chemistry_-_The_Central_Science_(Brown_et_al.)/11%3A_Liquids_and_Intermolecular_Forces/11.02%3A_Intermolecular_Forces). Accessed 21 Mar. 2025.

Flowers, Paul, et al. “Intermolecular Forces.” *Atoms First OpenStax*, OpenStax, 19 Oct. 2018,

pressbooks.nscc.ca/chemistryatoms/chapter/intermolecular-forces/. Accessed 21 Mar. 2025.

“Group 17: General Properties of Halogens.” *Chemistry LibreTexts*, Libretexts, 30 June 2023,

[chem.libretexts.org/Bookshelves/Inorganic_Chemistry/Supplemental_Modules_and_Websites_\(Inorganic_Chemistry\)/Descriptive_Chemistry/Elements_Organized_by_Block/2_p-Block_Elements/Group_17%3A_The_Halogens/0Group_17%3A_Physical_Properties_of_the_Halogens/Group_17%3A_General_Properties_of_Halogens#:~:text=the%20halogen%20group%3A-,Melting%20and%20Boiling%20Points%20\(increase%20down%20the%20group\),the%20van%20der%20Waals%20forces](http://chem.libretexts.org/Bookshelves/Inorganic_Chemistry/Supplemental_Modules_and_Websites_(Inorganic_Chemistry)/Descriptive_Chemistry/Elements_Organized_by_Block/2_p-Block_Elements/Group_17%3A_The_Halogens/0Group_17%3A_Physical_Properties_of_the_Halogens/Group_17%3A_General_Properties_of_Halogens#:~:text=the%20halogen%20group%3A-,Melting%20and%20Boiling%20Points%20(increase%20down%20the%20group),the%20van%20der%20Waals%20forces). Accessed 21 Mar. 2025.

"Physical Constants of Organic Compounds." *CRC Handbook of Chemistry and Physics*, Internet Version 2005, edited by David R. Lide, CRC Press, 2005, <http://www.hbcpnetbase.com>.

"6.1: Physical Properties of Haloalkanes." *Chemistry LibreTexts*, Libretexts, 14 July 2020, [chem.libretexts.org/Bookshelves/Organic_Chemistry/Map:_Organic_Chemistry_\(Vollhardt_and_Schore\)/06._Properties_and_Reactions_of_Haloalkanes:_Bimolecular_Nucleophilic_Substitution/6-01_Physical_Properties_of_Haloalkanes](https://chem.libretexts.org/Bookshelves/Organic_Chemistry/Map:_Organic_Chemistry_(Vollhardt_and_Schore)/06._Properties_and_Reactions_of_Haloalkanes:_Bimolecular_Nucleophilic_Substitution/6-01_Physical_Properties_of_Haloalkanes). Accessed 21 Mar. 2025.

Monroe, Manus. "The Importance of Weak Forces." *RSC Education*, 29 July 2024, edu.rsc.org/feature/the-importance-of-weak-forces/2020255.article. Accessed 21 Mar. 2025.