CHEMISTRY INTERNAL ASSESSMENT

Investigating the effect of structural isomerism (positional, chain and metamerism) on the boiling points of aliphatic alcohols and ethers

Introduction

While learning about intermolecular forces in our Chemistry lessons, alcohols were taught as prime examples of hydrogen bonding between molecules. We learned that the boiling points of alcohols are significantly higher than hydrocarbons of comparable molar mass (e.g. alkanes or alkenes) because of the strong intermolecular hydrogen bonding present in alcohols. Alcohols find use in our everyday lives and in industries alike; for instance isopropyl alcohol (2-propanol) is commonly applied to the skin as an antiseptic, and is also an important component in lotions and other cosmetics. On the other hand, its isomer propyl alcohol (1-propanol) is largely used in industries as a solvent in pharmaceuticals and in the preparation of lacquers. Both compounds differ only by the position of the hydroxyl group on the carbon chain and yet they have widely different physical properties and thus find different uses. This concept led me to consider why such small changes in the structure of a molecule have a drastic impact on its properties and how intermolecular forces play a role in it.

The boiling point of a compound depends on the intermolecular forces that exist between its molecules. Alcohols are organic compounds characterized by the presence of a hydroxyl functional group (–OH) attached to an alkyl group on a hydrocarbon chain. The hydroxyl group is able to form hydrogen bonds, the strongest intermolecular forces, with hydroxyl groups present in other alcohol molecules. When oxygen, a highly electronegative atom, covalently bonds to a hydrogen atom within an alcohol molecule, it induces polarity in the molecule. A partially positive charge is formed on the hydrogen atom and a partially negative charge is formed on the oxygen atom. As a result of the high difference in electronegativity, the hydrogen atom in one molecule is highly electrostatically attracted to the oxygen atom in a neighboring alcohol molecule. The negatively polarized oxygen acts as a hydrogen bond acceptor, while the hydrogen attached to the oxygen serves as a hydrogen bond donor, forming a hydrogen bond. As there are both hydrogen bond acceptor and donor in the same molecule, a strong network of alcohol molecules is created in the liquid phase that requires more energy to break apart. This is why the boiling points of alcohols are significantly higher than that of alkanes of comparable molecular mass.

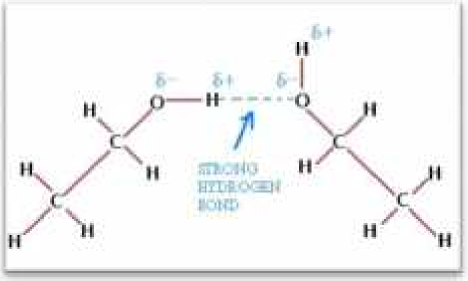


Figure 1: Formation of a hydrogen bond between ethanol molecules (n.d.)

In Chemistry lessons we also learned that increasing the carbon chain length of organic compounds increases its overall London dispersion forces, which increases the compound's boiling point. Following this, I wondered what factors could affect the other intermolecular forces found between molecules. Alcohols are the perfect homologous series to investigate in this regard as they exhibit all 3 IMFs; namely London dispersion forces, dipole-dipole forces and hydrogen bonding. Isomerism is the phenomenon in which different compounds have the same molecular formula but differ in their chemical structures. In this investigation, I will be looking at 3 types of structural isomerism; positional isomerism, chain isomerism and metamerism.

Positional isomerism

Positional isomerism is a type of structural isomerism in which each isomer differs in terms of position of the functional group on the carbon skeleton. In alcohols, the position of the hydroxyl group affects how exposed the surface of the oxygen atom is for hydrogen bonding with other alcohol molecules. Theoretically, as the functional group moves inwards on the carbon chain it becomes more shielded by the surrounding alkyl groups, which makes the oxygen atom less accessible to hydrogen atoms in neighbouring alcohol molecules, thus reducing the likelihood of forming a strong hydrogen bond. Hence isomers with the hydroxyl functional group more exposed and on the outside of the carbon chain should be having higher boiling points than isomers with the functional group less exposed and on the inside of the carbon chain.

Chain isomerism

Chain isomerism occurs due to branching of carbon chains on the main carbon skeleton. A straight chain organic compound has a higher surface area that allows for more Van der Waal interactions to take place between molecules, increasing the total strength of the IMFs and hence raising the boiling point. On the other hand, branching makes the molecule more compact, reducing the surface area available for Van der Waal interactions, and contributes to a lower boiling point.

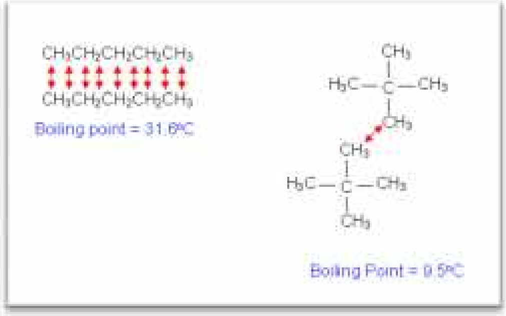


Figure 2: Van der Waals forces in an aliphatic vs. branched hydrocarbon

The effect of chain isomerism can be measured through solvent accessible surface area, as surface area is proportional to the Van der Waals forces of the molecule.

Metamerism

Ethers are isomers of alcohols with an ether functional group instead of hydroxyl, that consists of an oxygen atom forming single bonds with two alkyl groups and have the formula R-O-R'. Similar to alcohols, these compounds find use in production of dyes, perfumes, oils, waxes and other industries. The strongest intermolecular forces in ethers are dipole-dipole forces instead of the hydrogen bonds that are present in alcohols. As a result of this ethers possess significantly lower boiling points than alcohols of similar molecular mass. Due to high electronegativity of the oxygen atom along with the lone pair of electrons it possesses, the shared pair of electrons between the alkyl groups and the ether functional group is pulled more tightly towards the oxygen atom, forming a dipole moment ("Dipole Moments"). Because of the lone pair of electrons on the oxygen atom, the overall molecular geometry of ether molecules are bent (via VSEPR theory) which means that the vectors representing the dipole moment do not cancel each other out, giving the molecule a net dipole moment.

Figure 3: Dipole moment in an ether molecule ("Names and Properties of Ethers")

Metamerism is a type of functional isomerism that ethers exhibit where molecules with the same chemical formula have different alkyl groups attached on either side of the functional group, for example consider the structures of diethyl ether and methyl propyl ether, both which have the molecular formula of $C_4H_{10}O$. Diethyl ether has an ethyl group on either side of the functional group while methyl propyl ether has a propyl group on one side and a methyl group on the other.

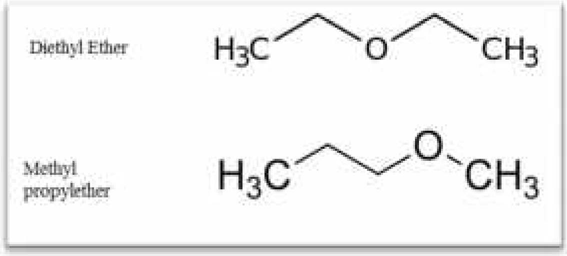


Figure 4: Example of metamerism in two ether isomers of $C_4H_{10}O$

It is also important to note that positional isomerism is different from metamerism; in positional isomerism the functional group is attached to different positions on the carbon chain whereas in metamerism, different alkyl groups are attached to the same functional group.

A symmetrical ether molecule reduces its polarity to some extent by balancing the negative charge among the atoms through an inductive effect, but in an asymmetrical molecule the charge is shared unequally which causes a higher dipole moment. Due to this, asymmetrical ethers with different alkyl groups on each side of the functional group would be expected to have a higher boiling point than a symmetrical metamer of comparable molecular weight. The larger the difference between the sizes of the alkyl groups joined to the oxygen atom, the higher the dipole moment and the higher the boiling point.

Research Questions

1. What is the effect of positional isomerism on the boiling points (in °C) of aliphatic alcohols?
2. What is the effect of branching on the boiling points (in °C) of aliphatic alcohols as measured by Van der Waals surface area (in Å)?
3. What is the effect of metamerism on the boiling points (in °C) of aliphatic ethers as measured by dipole moments (in Debyes)?

<u>Variables</u>

<u>Part 1: Positional isomerism and boiling points</u>

Independent variable: The position of the hydroxyl group on the carbon chain.

Dependent variable: Boiling point of the aliphatic alcohol in °C.

<u>Part 2: Chain isomerism and boiling points</u>

Independent variable: Solvent accessible surface area of the branched alcohol in Angstroms.

Dependent variable: Boiling point of the isomeric alcohol in °C.

<u>Part 2: Metamerism and boiling points</u>

Independent variable: Overall dipole moment of the ether in Debyes.

Dependent variable: Boiling point of the ether in °C.

In order to ensure that the results of this investigation are as reliable and accurate as possible, certain confounding variables had to be accounted for. These are summarized in the following table.

Table 1: Control variables

Control Variable	Significance	How it will be controlled
Shape of the molecule	Branching in molecules affects its boiling point.	Only straight-chained alcohols and ethers were analyzed for research questions 1 & 3.
Position of hydroxyl group on the carbon chain	Position of the hydroxyl group can affect the boiling point of the compound via shielding effects.	Branched alcohols with the hydroxyl group on the first carbon atom on the carbon chain were used for analysis for research question 2.

As this is a database investigation, there are no ethical, environmental or safety considerations.

Sources

To answer the research questions, data will be sourced from the following databases, which were selected on basis of their credibility and reliability:

1. The NIST Chemistry WebBook providing access to data compiled and shared by the National Institute of Standards and Technology, an agency under the US Department of Commerce.
2. The 85th edition of the CRC Handbook of Chemistry and Physics, a trusted reference source for reliable Chemistry data.
3. The PubChem Online Database maintained by the National Center for Biotechnology Information and approved by the government of the United States.
4. The ChemSpider Online Database, run by the Royal Society of Chemistry.
5. The Chemicalize Online Database run by ChemAxon, a cheminformatics company.
6. WebMO, a web-based 3D computational molecular modeling program.

Experimental data for boiling points was sourced from the first 4 databases, while ChemAxon and WebMO were used for solvent accessible surface area data for branched alcohols and dipole moment data for ethers respectively. For boiling points, the NIST WebBook was my first choice due to the availability of data for a wide range of compounds on the site, and its reliability as it is run by a reputable organization and has been used as a data source in many published papers. Additionally, the uncertainties of most of the boiling point data were clearly stated which was helpful in assessing the reliability of each value. The CRC Handbook contains data for most molecules in study and was my second choice due to how popular a reference source it is in chemistry research. Lastly, PubChem and Chemspider allowed me to get a comprehensive view of all isomers of a given molecular formula; however they had inconsistent data for the compounds I required and hence were my last choices.

Methodology

Data for boiling points was extracted from the respective databases for all isomers there was consistent data for across all databases. As enough boiling point data for many molecules wasn't available to give a reliable average, my analysis was restricted with regards to the number of isomers analyzed in each research question. There was the option of using computationally predicted boiling point data, but I was doubtful about their reliability as compared to experimental data.

Data for all isomers within the given ranges were extracted from the chosen sources and logged onto Excel for processing; values for boiling points were taken on an average of 4 data points to account for error variability and improve accuracy of the results. The values thus obtained were then plot on a line graph to visually observe the data and analyze any trends.

Apart from the NIST database the specific calculation methods used in each database were not stated, as a result this investigation was unable to account for the uncertainties that may have arisen in each databases' calculation process. For databases for which this information was not available, it was assumed that the method of calculation was perfectly accurate, thus the uncertainties correspond to the last decimal place of the value to account for the effect of rounding.

Analysis

Part 1

For question 1 all isomeric alcohols from C_4H_9OH to $C_8H_{17}OH$ were chosen for analysis as only molecules with 4 or more carbons can exhibit chain isomerism, and data beyond $C_8H_{17}OH$ was not consistently available throughout all databases to give a reliable average of boiling point. All isomers selected had the hydroxyl group on the 1st carbon and branching occurring on the 2nd carbon followed by the 3rd carbon in bigger molecules to control for the effect of positional isomerism on the boiling points.

Table 2: Boiling points of the positional isomers of 11 aliphatic alcohols

Formula	Isomers	Molecular weight (in g/mol)	Structural formula	Boiling points (in °C)				Average boiling point (in °C)
				PubChem (±0.1)	ChemSpider (±0.1)	CDC (±0.1)	NIST	
C_3H_8O	**1-Propanol**	60.10		97.2	97.0	97.2	97.2 ±0.1	97.1
	2-Propanol			82.3	82.0	82.3	82.4 ±1.7	82.2
$C_4H_{10}O$	**1-Butanol**	74.12		117.5	117.5	117.3	117.5 ±0.2	117.4
	2-Butanol			99.5	98.0	99.51	98.9 ±0.1	99.0
$C_5H_{12}O$	**1-Pentanol**	88.15		137.8	137.0	138.0	137.9 ±0.3	137.7
	2-Pentanol			119.2	117.4	119.3	118.9 ±0.3	118.7
	3-Pentanol			116.1	114.5	116.3	114.9 ±0.6	115.4
$C_6H_{14}O$	**1-Hexanol**	102.17		157.0	157.0	157.6	156.9 ±1.3	157.1
	2-Hexanol			136.0	137.0	140.0	137.9 ±1.0	137.7
	3-Hexanol			-	134.5	135.0	133.9 ±0.7	134.5
$C_7H_{16}O$	**1-Heptanol**	116.20		175.7	175.5	176.5	174.9 ±0.8	175.6
	2-Heptanol			159.0	159.7	159.0	158.9 ±1.1	159.1
	3-Heptanol			-	157.3	157.0	152.0 ±1.1	155.4
	4-Heptanol			156.0	156.5	156.0	154.9 ±0.7	155.8
$C_8H_{18}O$	**1-Octanol**	130.23		194.8	194.4	195.2	194.9 ±0.4	194.8
	2-Octanol			178.9	179.0	179.3	177.6 ±0.1	178.7
	3-Octanol			-	174.7	171.0	175.0 ±0.1	173.6
	4-Octanol			-	175.0	176.3	176.0 ±0.8	175.8
$C_9H_{20}O$	**1-Nonanol**	144.25		214.1	213.3	213.4	211.9 ±3.9	213.2
	2-Nonanol			193.5	194.8	193.5	195.9 ±2.1	194.4
	3-Nonanol			-	193.0	195.0	194.8 ±1.2	194.3

	4-Nonanol			-	193.5	192.5	192.5 ±1.2	192.8
	5-Nonanol			193.0	195.0	193.0	195.1 ±0.1	194.0
$C_{10}H_{22}O$	**1-Decanol**	158.28		230.0	232.0	231.1	231.9 ±1.4	231.2
	2-Decanol			-	211.0	211.0	211.1 ±0.1	211.0
	3-Decanol			-	213.0	213.0	211.1 ±0.6	212.4
	4-Decanol			-	210.5	210.5	210.6 ±0.1	210.5
	5-Decanol			-	-	201.0	389.9 ±0.6	295.4
$C_{11}H_{24}O$	**1-Undecanol**	172.31		243.0	243.0	245.0	-	244.0
	2-Undecanol			-	227.0	229.7	229.9 ±1.8	228.9

1C represents all isomers with the hydroxyl group on the first carbon atom, 2C with the hydroxyl group on the second carbon atom and so on.

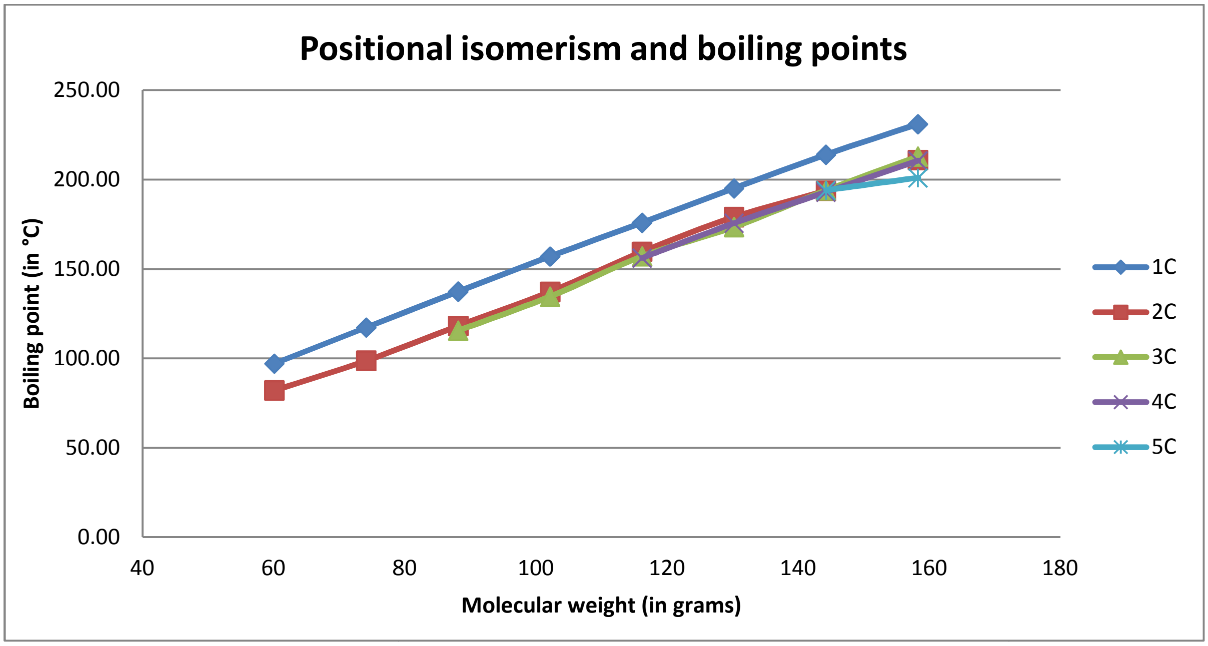


Figure 5: Change in boiling points as the position of the hydroxyl group changes

A considerable drop can be observed in the boiling point from molecules with the hydroxyl group on the first carbon to the second carbon. A very slight difference can also be observed between the boiling points of 2C and 3C hydroxyl alcohols. This difference becomes less significant as we start moving the –OH group to higher carbon numbers, and the boiling points start to merge.

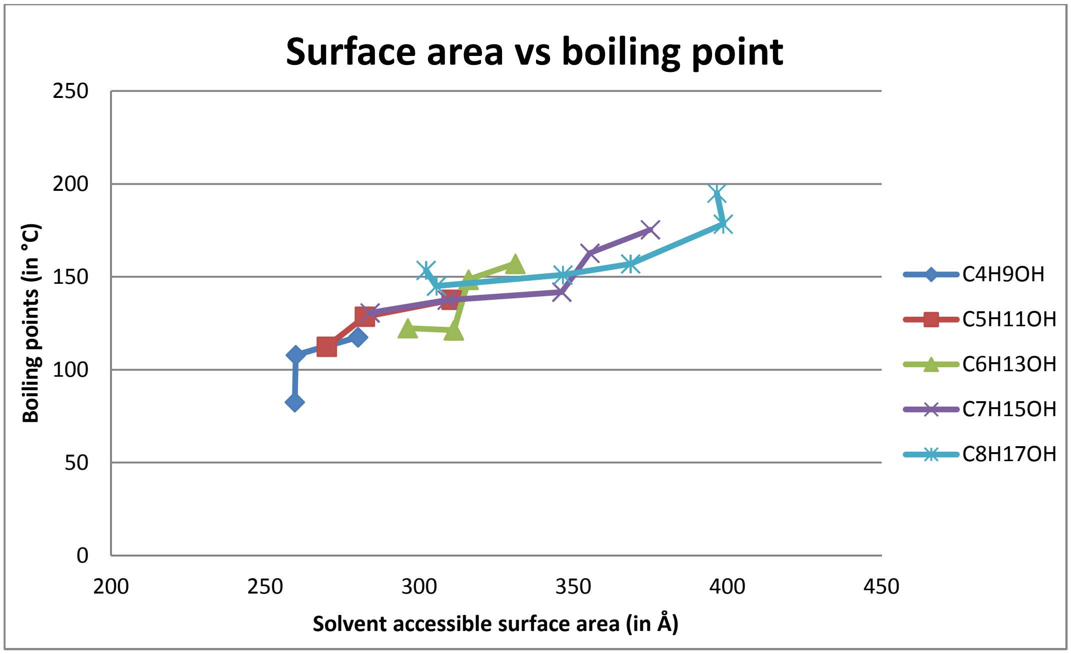
This is probably because the oxygen atom is most exposed and thus accessible to other hydroxyl groups when it is at the lowest carbon atom, and when it moves further inwards to a 2-carbon the hydroxyl group experiences shielding by the two alkyl groups on its sides. This shielding effect increases as the –OH group moves even further in the carbon atom to 3C isomers, and then converges at the 4C and 5C molecule probably because only the two alkyl groups on the sides of the functional group have a significant shielding effect, and this remains constant in all positional isomers except the 1C isomer, which is why the boiling point also converges accordingly. However, the 5C carbon isomer at 158.28g does not fit this prediction with its boiling point being lower than the corresponding 4-carbon and 3-carbon molecules of the same molecular mass. Upon analyzing the structures of the two molecules using ChemSketch (a chemical molecule visualization software) I think that this is not due to inherent differences between the structures of the molecules but due to errors in the data values for 5-decanol, as only two values were used to calculate the average boiling point for this molecule which likely caused more error variability as the two values have a large difference between them (389.9°C and 201.0°C respectively).

Part 3

Solvent accessible surface area is a geometric measure of how exposed a molecule is in a particular solvent (Durham). As London dispersion forces are directly proportional to surface area of the molecule, solvent accessible surface area was used as a measure of the London forces in each molecule.

Table 3: Values for solvent accessible surface area (in Å) and boiling points (in °C) of branched alcohols

IUPAC name	**Skeletal formula**	**Boiling points (in °C)**					**Solvent Accessible Surface area (in Å)**
		PubChem (±0.1)	**ChemSpider (±0.1)**	**CDC (±0.1)**	**NIST**	**Average**	
C_4H_9OH							
1-Butanol		117.5	117.5	117.3	117.5 ±0.01	117.5 ±0.1	280.1
2-Methyl-1-propanol		108.0	108.0	107.9	107.7 ±0.3	107.9 ±0.3	259.9
2-Methyl-2-propanol		82.4	83.0	82.4	82.4 ±0.2	82.6 ±0.2	259.6
$C_5H_{11}OH$							
1-Pentanol		137.8	137.0	138.0	137.9 ±0.3	137.7 ±0.3	310.5
2-Methyl-1-butanol		128.0	130.0	127.5	128.9 ±0.6	128.6 ±0.6	282.3
2,2-Dimethyl-1-propanol		113.5	112.0		111.9 ±0.9	112.5 ±0.9	270.0
$C_6H_{13}OH$							
1-Hexanol		157.0	157.0	157.6	156.9 ±0.7	157.1 ±0.7	331.1
2-Methyl-1-pentanol		149.0	148.0	149.0	147.9 ±0.7	148.5 ±0.7	315.9
2-Methyl-2-pentanol		121.1	121.0	121.1	121.9 ±0.6	121.3 ±0.6	311.2
3-Methyl-3-pentanol		122.4	123.0	122.4	121.9 ±0.6	122.4 ±0.6	296.2
$C_7H_{15}OH$							
1-Heptanol		175.7	175.5	176.5	174.9 ±0.8	175.4 ±0.8	374.9
2-Methyl-1-hexanol		-	161.3	164.0	162.9 ±1.5	162.7 ±1.5	355.3
2-Methyl-2-hexanol		-	141.5	143.0	140.9 ±1.0	141.8 ±1.0	346.3
2,3-Dimethyl-2-pentanol		-	-	-	137.5 ±1.0	137.5 ±1.0	309.8
2,3,3-Trimethyl-2-butanol		131.0	-	131.0	129.9 ±1.0	130.6 ±1.0	284.7
$C_8H_{17}OH$							
1-Octanol		194.8	195.0	195.2	194.9 ±0.4	195.0 ±0.4	396.5
2-Methyl-1-heptanol		179.3	179.0	175.6	179.9 ±0.4	178.4 ±0.4	398.6
2-Methyl-2-heptanol		156.0	-	156.0	158.9 ±2.2	157.0 ±2.2	368.5
2,3-Dimethyl-2-hexanol		-	-	-	151.0 ±0.7	151.0 ±0.7	346.6
2,3,3-Trimethyl-2-pentanol		-	145.0	-	-	145.0 ±0.1	305.5
2,2,3-Trimethyl-3-pentanol		-	-	-	153.5 ±1.1	153.5 ±1.1	302.2



It is worth noting that as the chain length increases, the differences in boiling point become lower with increasing branching. This is because as the chain length increases, the molecule becomes more rod-like rather than spherical despite branching. For example, comparing 2-Methyl-2-propanol and 2,2,3-Trimethyl-3-pentanol.

Part 3

To quantify the effect of metamerism on the dipole-dipole forces of the ether molecules, dipole moment was calculated, which is a measure of the polarity of a molecule. To calculate this, molecular modeling on the online computational chemistry program WebMO was used following the steps below.

1. Create a new job and draw in the target molecule.
2. Click the ‘Cleanup’ tab and select ‘Comprehensive – Idealized’.

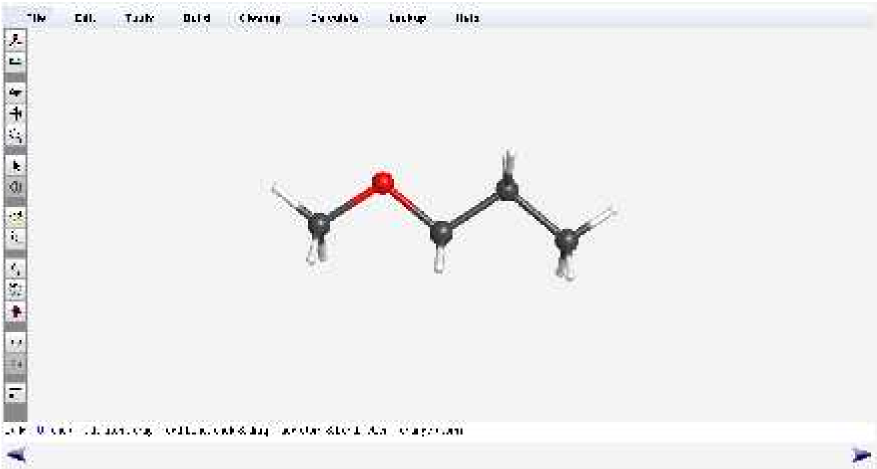


Figure 6: Building a 1-Methoxypropane molecule on WebMO

3. Go to the next page using the arrow on the right hand corner and select the ‘Gamess’ engine.
4. Under ‘Job Options’ set the calculation drop-down list to ‘Molecular Energy’ and go to the next page.

5. Once the calculation is done, open the target molecule and scroll down to 'Calculated Quantities' and record the overall dipole moment in Debyes under the 'Overview' tab.

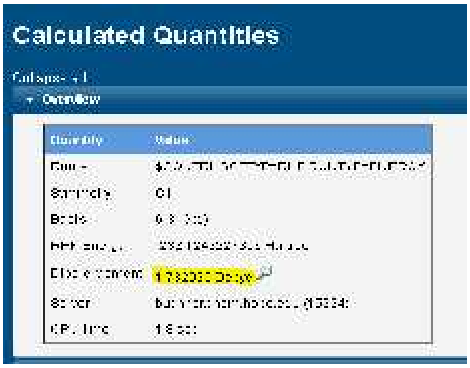
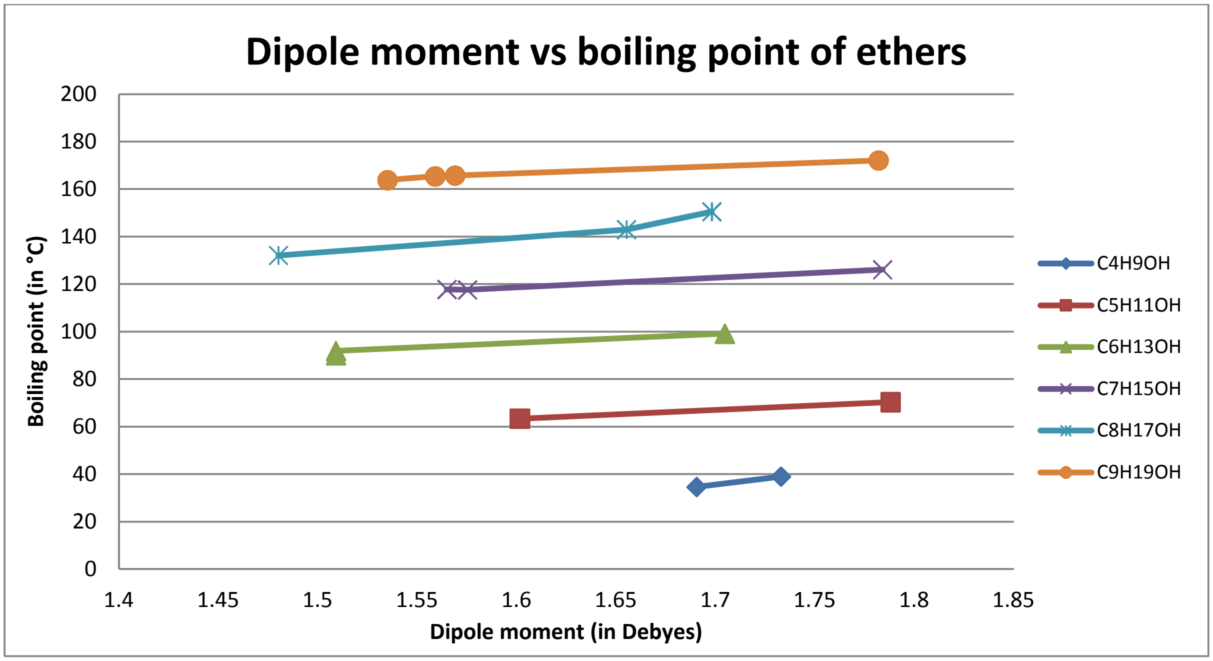


Figure 7: Dipole moment calculation for 1-Methoxypropane

This procedure was repeated for all 24 ethers and the data obtained is displayed as follows:

Table 4: Values for boiling points (in °C) and dipole moments (in Debyes) of each metamer from C4-C9

Molecular formula	IUPAC Name	Skeletal structure	Boiling point (in °C)						Dipole moment (in Debyes)
			PubChem (±0.1)	ChemSpider (±0.1)	CDC (±0.1)	NIST	ACD Labs	Average	
$C_4H_{10}O$	1-Methoxypropane		39.1	39	39.1	38.60 ±0.01	-	39.0 ±0.3	1.7329
	Ethoxyethane		34.6	34.6	34.5	34.60 ±0.02	-	34.6 ±0.3	1.6905
$C_5H_{12}O$	1-Methoxybutane		70.1	70.5	70.2	70.20 ±0.02	-	70.3 ±0.3	1.7880
	1-Ethoxypropane		63.2	-	63.2	63.70 ±0.02	-	63.4 ±0.2	1.6016
$C_6H_{14}O$	1-Methoxypentane		99.0	-	99.0	99.60 ±0.02	-	99.2 ±0.1	1.7047
	1-Ethoxybutane		92.3	91.5	92.3	91.55 ±0.03	-	91.9 ±0.3	1.5091
	1-Propoxypropane		90.0	90.5	90.1	89.90 ±0.20	-	90.1 ±0.5	1.5091
$C_7H_{16}O$	1-Methoxyhexane		126.1	126.1	126.1	126.10 ±0.10	-	126.1	1.7840
	1-Ethoxypentane		117.6	-	117.6	117.60 ±0.10	-	117.6	1.5752
	1-Propoxybutane		118.1	-	118.1	117.20 ±0.10	-	117.8	1.5649
$C_8H_{18}O$	1-Methoxyheptane		-	-	-	-	150.5 ±3.0	150.5	1.6981
	1-Ethoxyhexane		-	-	143.0	-	135.5 ±0.0	143.0	1.6552
	1-Propoxypentane		-	-	-	132.10 ±0.10	142.2 ±3.0	132.1	1.4801
	1-Butoxybutane		142.0	142.0	140.3	141.90 ±0.30	142.1 ±8.0	141.6	1.6204
$C_9H_{20}O$	1-Methoxyoctane		-	-	-	172.10 ±0.30	173.5 ±3.0	172.1	1.7823
	1-Ethoxyheptane		166.0	-	-	-	165.5 ±3.0	165.8	1.5693
	1-Propoxyhexane		-	-	-	-	165.4 ±3.0	165.4	1.5598
	1-Butoxypentane		-	-	-	-	163.8 ±8.0	163.8	1.5351



The above graph shows an increase in boiling points as the dipole moment increases in ether molecules. The greater the increase in polarity, the higher the increase in boiling point. There are a few metamers that do not adhere to this rule and have similar dipole moments despite having different alkyl groups on the side of the ether functional group, namely the third data point for $C_9H_{20}O$ and the second data points belonging to $C_7H_{16}O$ and $C_6H_{14}O$. Despite having different alkyl groups compared to the preceding metamer, the dipole moments and boiling points between the molecules do not differ by much.

Evaluation

As this was a database investigation, I was able to examine the effect of different types of structural isomerism on all 3 intermolecular forces in depth using a wide range of compounds which would have not been possible with the facilities of a normal school laboratory. I was also able to use technology to my advantage and understand chemistry phenomena better by exploring molecular modeling in this IA. However, there were several limitations to the current investigation; these have been summarized in the table below along with suggestions for improvements.

Table 5: Limitations of the study

Limitation	How it affected the investigation	Suggestions for improvement
Use of solvent accessible surface area to measure London dispersion forces	Solvent accessible surface area is a measure of the surface area of the molecule that can come into contact with the solvent sphere ("Molecular Surface Area"). As the analysis involves boiling point which involves overcoming the intermolecular forces of attraction, a 'solvent' is irrelevant to a compound's boiling point. Thus the assumption that the solvent accessible surface area is proportional to the London dispersion forces may not be accurate. Having said so, as the data for solvent accessible surface area was applied to all alcohols investigated, the area can be considered as a relative surface	Molecular modeling programs that calculate molecular surface area specifically can be used for data collection.

	area for comparison purposes.	
Number of compounds studied	As limited experimental data for boiling points were available online for isomers of each molecular formula, the number of compounds analyzed under each research question was limited. This could affect the overall conclusion and reliability of the findings as trends between a few structural formulas are being generalized across the homologous series.	Predicted boiling point data from computational chemistry programs such as EPISuite and ACDLabs available online could be used for analysis, although it is unclear how reliable this data is compared to experimentally obtained values.

Conclusion

This study aimed to answer the following question: **“How does structural isomerism affect the boiling points of alcohols and ethers?”** Overall, the initial hypotheses mentioned in the introduction were substantiated to some extent. The main conclusions gathered from the analysis of the data are as follows:

1. The position of the hydroxyl group on the carbon chain in an alcohol affects the accessibility of the oxygen atom to form hydrogen bonds and thus the boiling point increases when the hydroxyl group is closer to the 1st carbon on the carbon chain, as this is where the oxygen atom is least obstructed. On the other hand, when the hydroxyl group is positioned closer to the inside of the chain on a higher number carbon, the shielding effect of the surrounding alkyl groups reduces the strength of the hydrogen bond formed between the oxygen and another alcohol molecule. However this difference is only significant up to the 2nd carbon atom, as the shielding effect remains the same beyond this point.
2. The boiling point of alcohols lowers as the alcohol branches more, as this reduces the surface area available for London dispersion forces, resulting in weaker London forces between molecules and less energy is required to overcome these forces. Conversely, alcohols with less branching have more area available for London dispersion attractions to take place and thus higher boiling points.
3. Highly symmetrical ethers with identical alkyl groups on both sides have the lowest dipole moments due to inductive effect and thus the lowest boiling points. Furthermore, asymmetrical ethers with large difference between sizes of the two alkyl groups have a higher overall dipole as the charge is not distributed as effectively across the molecule, giving stronger dipole bonds and thus a higher boiling point.

As the differences between predicted and experimental data was one of the major caveats of this investigation, an extension could be looking at the percentage difference between experimentally obtained and predicted data to determine which is more accurate in predicting trends between boiling points in alcohols. Alternatively, lab experiments could be conducted to measure boiling points of some structural isomers of alcohol and compare them to predicted data, as this will help evaluate the validity of prediction tools as methods of data collection in chemistry research.

Furthermore, the present study only addressed the effect of structural isomerism in alcohols and ethers, the effect of structural isomerism in different functional groups can also be studied to see if the trends are consistent throughout different types of compounds.

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