# Modelling Vapor Pressure of Molecules with Intermolecular Forces

How does the polarizability and dipole moment of a primary straight-chained molecule affect its vapor pressure?

### Introduction

When I learned about intermolecular forces in class, and related them to trends in boiling points, I was delighted by how I could finally learn the reasons for why things behaved as they did. Before IB Chemistry, I was expected to memorize certain trends, but this hadn't been enough to satisfy my infinite curiosity; now, I could finally learn the reasons behind many of them. I enjoyed this particularly because I am a logic-oriented person and I like it when everything abides rules and reason.

Therefore, when I learned that acetone had a lower boiling point than ethyl acetate, during an intermolecular forces experiment, I was very surprised. I had been expecting the opposite, because acetone is more polar than ethyl acetate, and my understanding was that any minor differences in temporary dipole forces / London dispersion forces were negligible when there was dipole-dipole attraction or hydrogen bonds in play. Apparently, in this case, the London dispersion force was strong enough to make a difference.

Upon this discovery, I wanted to come up with a way to model the physical characteristics of chemicals based on their individual intermolecular forces, and hence determine the extent of the intermolecular forces' effects. That's why for my Chemistry IA, I will be investigating the relationship between the relative strengths of the intermolecular forces in a substance, and its vapor pressure. After developing my model with a certain set of molecules, I will then test its applicability on other molecules.

### **Intermolecular Forces**

There are three major intermolecular forces that act on molecules:

### London Dispersion Force

Also known as the temporary dipole force, this is a relatively weak force that is present in all molecules, regardless of their structures and bonding. It "results when the electrons in two adjacent atoms [or molecules] occupy positions that make the atoms [or molecules] form temporary dipoles" (Purdue University). Larger molecules with more electrons experience stronger London dispersion forces.

### Dipole-Dipole Attraction

This is a significantly stronger force than the temporary dipole force. It occurs between polar molecules, because of their permanent dipoles. The more polar a molecule, the stronger the force.

### Hydrogen Bonding

Hydrogen bonding is the most substantial of the intermolecular forces. It is similar to dipole-dipole attraction, except that it only occurs when a hydrogen atom is bonded to an oxygen, nitrogen or fluorine atom, because the large difference in electronegativity will result in a very significant dipole.

### Vapor Pressure

The attraction caused by these forces is responsible for the vapor pressures of molecules. This is because when the attraction is greater, it takes more energy to move the molecules apart. As the vapor pressure is defined as "the equilibrium pressure of a vapor above its liquid" (Purdue University), it must decrease with increasing attractive forces, as fewer molecules will be in a gaseous state in equilibrium.

All of the vapor pressure values will be taken from the Royal Society of Chemistry's ChemSpider database. When possible, the experimental values which are attributed to NIOSH will be used. If the only experimental values on the ChemSpider page are from SynQuest, they will not be used, as they have shown to be very unreliable. For example, the SynQuest vapor pressure of ethene is 35 mmHg and that of butene is 37 mmHg, which are completely nonsensical values because they don't fit in with the rest of the data and because butene's vapor pressure should have been significantly smaller than ethene's. In the case of there being no appropriate experimental value, the ACD/Labs predicted value will be used.

The values will be expressed with two significant figures, and will be measured in millimeters of mercury. While the absolute uncertainties given by ChemSpider and the equivalent percentage uncertainties are different for each of the molecules, almost all of them lie between 0.1 and 0.9, which is why the uncertainty will be taken as the average, ±0.5 mmHg.

### Measuring Intermolecular Forces

If the three mentioned intermolecular forces can be quantified, they should then suffice to model the vapor pressures of molecules. In this case, they will be quantified by the polarizability and the net dipole moment.

### Polarizability

Polarizability is a measure of how easily electrons can move in response to an external field. London dispersion forces are directly proportional to polarizability, which is why this is an appropriate measure of that intermolecular force (University of Sydney).

The polarizability of a molecule depends on the number of electrons present, the size / surface area and the shape of the molecule. This investigation will focus on straight-chain molecules within the same homologous series, with varying numbers of carbon atoms but the same functional groups, so that the effect of the temporary dipole force on the vapor pressure can be observed clearly.

The predicted polarizability values will be taken directly from the ACD/Labs predicted values in the ChemSpider database. The only exception is methane, which is to be taken from the "Comparison of polarizabilities for LSDA/6-311G" table on the NIST website, as it isn't available on ChemSpider.

The values will be expressed in  $10^{-24}$  cm<sup>3</sup> and will have an uncertainty of  $\pm 0.5 \times 10^{-24}$  cm<sup>3</sup>.

### Dipole Moment

As both dipole-dipole attraction and hydrogen bonding are in effect the same thing, albeit of different strengths, they can be expressed together in the form of the net dipole moments of the molecules. The reason they shouldn't be measured and considered with two separate variables is because in certain molecules, they could act in opposite directions and cancel each other out; in this case, two scalar measurements for each of the forces might imply that the molecule has strong forces, even though they cancel each other out and have a weaker overall effect.

There are two other ways that could have been used to measure the strength of this polar attraction: the polarity index, or the polar surface area. However, the polarity index for many molecules is challenging to find, and the polar surface area is not sufficient because it only gives the surface area of the atoms in the molecule that form polar bonds, but does not consider just how polar the bonds are. Hence, the dipole moments are utilized instead.

It is difficult to find the dipole moments of most molecules, which is why a piece of software that can calculate and predict the value will be used. This is done frequently in literature, by using software such as MOPAC which utilizes molecular orbital theory (Yamamoto). In this investigation, version 14.6.4 of the Jmol software will be utilized as it is more user-friendly than MOPAC, and it is an open-source piece of software that is widely known and used; this means that it has been revised and improved over the many years it existed.

The following procedure will be used to extract the dipole moment values from Jmol:

- 1. Click on "File -> Get MOL" and type the molecule's name to load it.
- 2. Open the "Model Kit" toolbox, and click on "Fix Hydrogens and Minimize" to have Jmol recalculate and refresh the positions of the atoms, in case they aren't arranged correctly. It is best to do this two times, because when only done once, the dipole moment value can sometimes still be imprecise.

- 3. Launch the Jmol console and type the following commands (Hanson):
  - a. *dipole molecular* Calculates the dipole vector and draws it on the screen as an arrow.
  - b. **d** = getProperty("shapeInfo.Dipoles[1].vector") Assigns the dipole vector to variable 'd'.
  - c. **x** = sqrt(d\*d) Calculates the magnitude of the dipole by taking the dot product of the vector and finding its square root, and assigns it to variable 'x'.
  - d. *show variables* Displays the current values of the variables, including 'x', the dipole moment.



Figure 1, Pentanamide in JMOL with dipole moment vector

It should be noted that the unit of the dipole moment is the Debye, where 1 Coulomb-Meter is equal to  $2.9979 \times 10^{29}$  Debye. Furthermore, the calculated values are rounded to 2 decimal places, as the values appear to be more random beyond that. And finally, the resolution of these measurements – which was defined to be 2 decimal places, or 0.01 - will be taken as the uncertainty of the values.

### **Research Question**

How does the polarizability and dipole moment of a primary straight-chained molecule affect its vapor pressure?

# Hypothesis

I predict that the vapor pressure will be affected by the dipole-dipole attraction and hydrogen bonding more than the temporary dipole forces. That is, the dipole moment will have a bigger effect on the vapor pressure than the polarizability. Both of them will have an inverse relationship with the vapor pressure, because when they become larger, the intermolecular forces also become stronger, so the amount of molecules in gas form at equilibrium and thus the pressure they exert should decrease.

Furthermore, I believe that the effect of the temporary dipole force – which is expressed by polarizability – on the vapor pressure will be shaped as a negative exponential function, so that the differences in the vapor pressures will become smaller as the polarizability increases. This is because as the polarizability becomes larger, each additional increase by a constant value will yield a smaller percentage increase, and thus a smaller change of the vapor pressure. The reason I believe the graph will be a negative exponential and not a reciprocal function is because when the polarizability is zero, there are theoretically no intermolecular forces – assuming the molecule is non-polar and doesn't have hydrogen bonding – which means that the substance is completely in the gaseous state; hence, the vapor pressure would simply be equal to the gas's pressure in the

given conditions. Therefore, the curve should have a real y-intercept, and should look like a negative exponential function rather than a reciprocal.

# Variables

### **Independent Variables**

- Polarizability
- Dipole moment

The independent variables will be changed by examining a variety of molecules that possess different values.

The polarizability variable will be changed by looking at molecules of the same homologous series. As the number of carbon atoms increase, both the number of electrons and the surface area will also increase, which is why the polarizability will increase. The number of carbons for all the series will range from 1 to 10, except for the alkenes, alkynes and nitriles, which will start from 2.

The dipole moment will be changed by looking at different homologous series that range in both polarity and hydrogen bonding. The following series will be considered:

- Alkanes (C<sub>n</sub>H<sub>2n+2</sub>)
- Fluoroalkanes (C<sub>n</sub>H<sub>2n+1</sub>F)
- Chloroalkanes (C<sub>n</sub>H<sub>2n+1</sub>Cl)
- Bromoalkanes (C<sub>n</sub>H<sub>2n+1</sub>Br)
- Alkenes (C<sub>n</sub>H<sub>2n</sub>)
- Alcohols (C<sub>n</sub>H<sub>2n+1</sub>OH)
- Carboxylic acids (C<sub>n</sub>H<sub>2n+1</sub>COOH)
- Aldehydes (C<sub>n</sub>H<sub>2n</sub>O)
- Alkynes (C<sub>n</sub>H<sub>2n-2</sub>)
- Amides (C<sub>n</sub>H<sub>2n+1</sub>CONH<sub>2</sub>)
- Amines (C<sub>n</sub>H<sub>2n+1</sub>NH<sub>2</sub>)
- Nitriles (C<sub>n</sub>H<sub>2n-1</sub>N)

### **Dependent Variable**

The dependent variable will be the vapor pressure of the substance. It will be measured in millimeters of mercury, as this is the unit provided by the ChemSpider database.

### **Control Variables**

Only organic compounds belonging to homologous series will be used for the data, as other individual molecules would not fit in and wouldn't allow for a comparison with the polarizability the way molecules belonging to the same series do.

All the homologous series being considered in this investigation will be straight-chain series. Furthermore, they will all have their functional group bonded to their first carbon atom, meaning that they are primary compounds; this is why ketones or esters won't be considered.

And finally, temperature will be controlled. All of the vapor pressure values will be at 25 degrees Celsius, as that is how they are given on the ChemSpider database.

# Polarizability, Dipole Moment and Vapor Pressure of Molecules

Molecule	Polarizability	Dipole Moment	Vapor Pressure
	(±0.5 10 <sup>-24</sup> cm <sup>3</sup> )	(±0.01 Debye)	(±0.5 mmHg)
Methanol	3.3	2.23	96
Ethanol	5.1	2.24	44
Propanol	6.9	2.24	15
Butanol	8.8	2.24	6.0
Pentanol	10.6	2.24	2.8
Hexanol	12.4	2.25	0.9
Heptanol	14.3	2.25	0.3
Octanol	16.1	2.25	0.1
Nonanol	18.0	2.25	0.0
Decanol	19.8	2.25	0.0
Methanoic acid	3.3	5.49	35
Ethanoic acid	5.1	1.51	11
Propanoic acid	6.9	1.49	3.0
Butanoic acid	8.8	1.50	1.4
Pentanoic acid	10.6	1.48	0.5
Hexanoic acid	12.5	1.48	0.2
Heptanoic acid	14.3	1.49	0.1
Octanoic acid	16.1	1.49	0.0
Nonanoic acid	18.0	1.49	0.0
Decanoic acid	19.8	1.49	0.0
Methane	2.0	0.00	210,000
Ethane	4.5	0.00	29,000
Propane	6.3	0.00	7,300
Butane	8.2	0.00	1,600
Pentane	10.0	0.00	420
Hexane	11.8	0.00	120
Heptane	13.7	0.00	45
Octane	15.5	0.00	10
Nonane	17.3	0.00	3.0
Decane	19.2	0.00	1.6
Ethene	4.2	0.00	43,000
Propene	6.2	0.18	8,500
Butene	8.1	0.18	2,200
Pentene	9.9	0.18	640
Hexene	11.7	0.18	190
Heptene	13.6	0.18	57
Octene	15.4	0.18	18
Nonene	17.2	0.18	5.8
Decene	19.1	0.18	1.9
Fluoromethane	2.7	2.22	21,000
Fluoroethane	4.6	2.22	6,000
Fluoropropane	6.4	2.22	1,800
Fluorobutane	8.2	2.22	570
Fluoropentane	10.1	2.22	180
Fluorohexane	11.9	2.22	61
Fluoroheptane	13.7	2.22	20
Fluorooctane	15.6	2.22	7.1
Fluorononane	17.4	2.22	2.5
Fluorodecane	19.2	2.22	0.9
Chloromethane	4.6	2.47	3,800
Chloroethane	6.4	2.48	1,000
Chloropropane	8.2	2.48	340

Molecule	Polarizability	Dipole Moment	Vapor Pressure
	(±0.5 10 <sup>-24</sup> cm <sup>3</sup> )	(±0.01 Debye)	(±0.5 mmHg)
Chlorobutane	10.1	2.48	100
Chloropentane	11.9	2.48	32
Chlorohexane	13.8	2.48	10
Chloroheptane	15.6	2.48	3.3
Chlorooctane	17.4	2.48	1.1
Chlorononane	19.3	2.48	0.4
Chlorodecane	21.1	2.48	0.1
Bromomethane	5.7	2.15	1400
Bromoethane	7.6	2.16	380
Bromopropane	9.4	2.16	130
Bromobutane	11.2	2.16	40
Bromopentane	13.1	2.16	13
Bromohexane	14.9	2.16	4.0
Bromoheptane	16.7	2.16	1.3
Bromooctane	18.6	2.16	0.5
Bromononane	20.4	2.16	0.2
Bromodecane	22.2	2.16	0.1
Methanamide	4.1	4.33	0.2
Ethanamide	5.7	4.33	62
Propanamide	7.5	4.32	18
Butanamide	9.6	4.32	0.1
Pentanamide	11.4	4.33	0.1
Hexanamide	13.2	4.33	0.0
Heptanamide	15.1	4.32	0.0
Octanamide	16.9	4.33	0.0
Nonanamide	18.8	4.33	0.0
Decanamide	20.6	4.32	0.0
Methylamine	4.1	1.89	2,300
Ethylamine	5.9	1.88	870
Propylamine	7.7	1.88	330
Butylamine	9.6	1.88	82
Pentylamine	11.4	1.88	29
Hexylamine	13.2	1.88	9.1
Heptylamine	15.1	1.88	2.9
Octylamine	16.9	1.88	0.9
Nonylamine	18.7	1.88	0.3
Decylamine	20.6	1.88	0.1
Ethanenitrile	4.5	4.50	73
Propanenitrile	6.3	4.51	35
Butanenitrile	8.1	4.51	14
Pentanenitrile	10.0	4.51	5.8
Hexanenitrile	11.8	4.51	2.0
Heptanenitrile	13.6	4.51	0.7
Octanenitrile	15.5	4.51	0.2
Nonanenitrile	17.3	4.51	0.1
Decanenitrile	19.1	4.51	0.0
Methanal	2.6	3.68	760
Ethanal	4.6	3.76	740
Propanal	6.4	3.75	300
Butanal	8.2	3.75	96
Pentanal	10.1	3.75	26
Hexanal	11.9	3.75	11
Heptanal	13.7	3.75	3.9
Octanal	15.6	3.75	2.1

Molecule	Polarizability (±0.5 10 <sup>-24</sup> cm <sup>3</sup> )	arizability Dipole Moment Vap 5 10 <sup>-24</sup> cm <sup>3</sup> ) (±0.01 Debye) (±	
Nonanal	17.4	3.75	0.5
Decanal	19.3	3.75	0.2
Ethyne	3.6	0.00	34,000
Propyne	5.5	0.50	4,000
Butyne	7.3	0.50	1,400
Pentyne	9.1	0.50	430
Hexyne	11.0	0.50	130
Heptyene	12.8	0.50	44
Octyne	14.6	0.50	14
Nonyne	16.5	0.50	4.9
Decyne	18.3	0.50	1.7

Table 1, Polarizability, dipole moment and vapor pressure of molecules

### Legend:

Vapor Pressure:

Black = ACD/Labs Predicted Value from ChemSpider

Blue = NIOSH Experimental Value from ChemSpider Polarizability:

Black = ACD/Labs Predicted Value from ChemSpider Red = Predicted Value from NIST

# Analysis

The following graph is of vapor pressure vs polarizability. The different homologous series have each been represented by a different series of data / color. A logarithmic scale with base 10 has been used for the vapor pressure because of the large order differences between the series – ranging from 210,000 to 0.1. The error boxes for the uncertainties haven't been included, to keep the diagram legible.



Graph 1, Logarithmic chart of vapor pressure vs polarizability with different homologous series

As seen in the graph, one obvious outlier in the data is the vapor pressure of methanamide, which is much smaller than that of ethanamide, rather than being larger as expected. However, similar values were found on other online sources, such as the PubChem database by NIH, the NIOSH database by CDC, and ChemicalBook. This could mean that for some reason, the intermolecular forces of methanamide are unexpectedly strong. On the other hand, both the melting and boiling point of methanamide are smaller than those of ethanamide and the other amides, which does follow the expected trend and show that its intermolecular forces aren't necessarily stronger.

All of the homologous series except for the amides have a very clear and well-defined trend. The vapor pressure decreases as polarizability increases, as expected. Also, the more polar series such as carboxylic acids and alcohols have lower vapor pressures. This shows that this data is indeed answering the research question and appears to confirm the hypothesis.

Graph 2 is a polarizability vs. vapor pressure graph of only the alkanes. In this graph, a linear y-axis scale is used. This was done so that the relationship between these two variables would be more clear. There is clearly a negative exponential trend between polarizability and vapor pressure. Additionally, the trend curve is within the error bars, indicating a good fit.



Graph 2, Vapor pressure vs polarizability of alkanes

The average dipole moment must now be introduced into the calculations. A graph of vapor pressure vs dipole moment can't be plotted, as the polarizability values can't be kept constant. However, the dipole moment can instead be incorporated with the vapor pressure vs polarizability trend equations to develop a combined model that uses both polarizability and dipole moments together to predict vapor pressures, as explained below.

Homologous Series	Vapor Pressure vs	R <sup>2</sup> Value	Average Dipole	
	Polarizability Trend Equation		Moment	
Alkanes	$y = 594289e^{-0.697x}$	0.9952	0.00	
Alkenes	y = 541777e <sup>-0.668x</sup>	0.9982	0.16	
Alkynes	y = 188097e <sup>-0.647x</sup>	0.9925	0.44	
Fluoroalkanes	y = 92777e <sup>-0.608x</sup>	0.9992	2.22	
Chloroalkanes	y = 59218e <sup>-0.626x</sup>	0.9994	2.48	
Amines	$y = 32509e^{-0.618x}$	0.9995	1.88	
Bromoalkanes	$y = 32245e^{-0.59x}$	0.996	2.16	
Aldehydes	y = 5931.7e <sup>-0.527x</sup>	0.9882	3.74	
Nitriles	y = 979.57e <sup>-0.533x</sup>	0.9963	4.51	
Alcohols	y = 638.09e <sup>-0.534x</sup>	0.9973	2.24	
Carboxylic acids	y = 158.62e <sup>-0.531x</sup>	0.9917	1.89	
Amides	$y = 47.751e^{-0.477x}$	0.193	4.33	

Table 2 below lists each of the homologous series, along with the trend equations found from Graph 1, their respective R<sup>2</sup> values, and the average dipole moment of the first 10 molecules in that given series.

Table 2, Overview of data for different homologous series, sorted by decreasing trend equation coefficients

The trend equations for vapor pressure vs polarizability in Table 2 are all in the same exponential form, composed of a coefficient and a power:

$$y = Ae^{Bx}$$
 (Equation 1)

where A is the coefficient, B is the power, y is vapor pressure and x is polarizability.

As the vapor pressure vs polarizability trend equations for each of the homologous series are known, and the only values that vary in between these equations are A and B, these two values can then be modelled by the average dipole moments of the series. Hence, a model can be reached that uses both the polarizability and the dipole moment together to estimate the vapor pressure.



Graph 3 shows the effects of changing the dipole moment – by considering the different homologous series – on the coefficients and powers of the prior vapor pressure vs polarizability trend equations.

Graph 3, Coefficient and power of exponential trend equations vs dipole moment

The correlation between the dipole moments, and the coefficients and powers appear weak, with low R<sup>2</sup> values – 0.7331 and 0.5439. This indicates that the effect of the dipole moment is less clearly defined than that of polarizability, as that had high R<sup>2</sup> values around 0.99, listed in Table 2. However, there are still visible trends in the graph above, which is why the best fit equations may be used. It should be noted that this will be a significant source of error for the model.

The two trend equations found in Graph 3 can be substituted into Equation 1, and then simplified to get:  $y = (360454e^{-1.564*d}) * e^{(0.0385*d - 0.6716)*p} = 360454e^{-1.564*d + 0.0385*d*p - 0.6716*p}$ (Equation 2)

where y is vapor pressure, p is polarizability and d is the dipole moment.

### **Testing the Model**

The model was used to predict vapor pressures for each of the molecules in Table 1. The percentage errors were calculated with 100 \* |P - A| / A where P is the predicted value and A the actual value. The mean percentage errors for each of the homologous series is shown in Table 3. A sample calculation follows.

Homologous Series	Mean Percentage Error
Alkynes	13%
Alkanes	22%
Amines	26%
Alkenes	46%
Nitriles	52%
Bromoalkanes	60%
Chloroalkanes	75%
Aldehydes	81%
Fluoroalkanes	84%
Alcohols	970%
Amides	6100%
Carboxylic acids	9300%

Table 3, Mean percentage errors of vapor pressure for different homologous series, sorted by increasing errors

Sample Calculation with Methanoic Acid:

Polarizability = 3.3 Dipole Moment = 5.49 Actual Vapor Pressure = 35  
Vapor Pressure = 
$$y = 360454e^{-1.564*5.49+0.0385*5.49*3.3-0.6716*3.3} \cong 14.7$$
  
Percent Error =  $100 * \frac{|14.7-35|}{35} = 58\%$ 

In Table 3, most of the series have reasonable mean percentage errors, indicating that the predicted vapor pressures for those series are in the same order as the actual values. The only series that have significant errors are the alcohols, amides and carboxylic acids.

The model is also tested with molecules that were not used earlier in the investigation, to see how well it applies to new molecules. The molecules were chosen such that one is not primary (3-heptylamine), one is from a homologous series that wasn't used (2-pentanone), one has a branched chain (4-octyne), one is cyclic (methylbenzene), one is inorganic (tetrafluorosilane), and one is a diatomic element (chlorine). The results are shown in Table 4:

Molecule	Polarizability	Dipole Moment	Predicted Vapor	Actual Vapor	Error
			Pressure	Pressure	
3-Heptylamine	15.1	1.86	2.3	5.0	54%
2-Pentanone	10.0	3.81	4.9	27	82%
4-Octyne	14.7	0.00	19	11	69%
Methylbenzene	12.3	0.24	72	21	240%
Tetrafluorosilane	4.5	0.00	18000	26000	32%
Chlorine	4.7	0.00	15000	5200	200%

Table 4, Comparison of real and predicted vapor pressures of new molecules

# **Conclusion and Evaluation**

In this investigation, the effect of polarizability and net dipole moment on the vapor pressure of primary straight-chained molecules was explored. A model that predicts vapor pressure was developed and tested. It was found that both of the independent variables have a negative relationship with the dependent variable. This can be seen in Graph 1, where increasing polarizabilities yield decreasing vapor pressures, and homologous series with larger dipole moments have smaller vapor pressures. This finding is consistent with the relevant scientific context, as increasing intermolecular forces should indeed be decreasing the vapor pressure.

There were two hypotheses presented in the beginning of the investigation. The first was that the dipoledipole attraction and hydrogen bonding, both represented by the dipole moment, would have a stronger impact on the vapor pressure than the temporary dipole force, which is represented by polarizability, and that both would have an inverse relationship with the vapor pressure. It can be seen that the data supports this hypothesis, by inspecting Equation 2:

$$v = 360454e^{-1.564*d + 0.0385*d*p - 0.6716*p}$$

The coefficient of the dipole moment (-1.564) is greater in magnitude than that of polarizability (-0.6716), indicating that it has a more distinct impact. Additionally, both coefficients are negative, resulting in a decrease of vapor pressure when either the dipole moment or the polarizability increases, which indicates an inverse relationship. This confirms the first hypothesis.

The second hypothesis was that the polarizability would affect the vapor pressure in the shape of a negative exponential function. By comparing the R<sup>2</sup> values, it was found that the negative exponential function modelled the data the best, so this hypothesis is also supported by the data.

The model had reasonably small percentage errors for most of the homologous series. Alcohols, amides and carboxylic acids had very large errors; this could be related to the fact that all three series have hydrogen bonding. In the investigation, the dipole moment was assumed to be a reasonable measure of both the dipoledipole attraction and hydrogen bonding, but this may have not been the case, resulting in significant errors. It can therefore be concluded that either the dipole moment as a concept doesn't account for hydrogen bonding, or JMOL doesn't do so when computing the dipole moments. It is more likely to be the latter, as the electronegativity differences in hydrogen bonds should be producing dipole moments. The investigation could therefore be improved by either using a program that correctly incorporates hydrogen bonding, such as the hydrogen bond enthalpy. The only problem with this conclusion is that although the amines also have hydrogen bonding, they actually had much smaller percentage errors. These occurrences could therefore be an area of focus for future studies.

When tested on new molecules, the model performed reasonably well. This shows that despite the limited number of molecules used to develop it, the model can still extrapolate its predictions to new molecules. The model could be further improved by incorporating other molecules when developing it. The number of molecules used per homologous series – nine to ten – was sufficient, as the last molecule of each series had a vapor pressure close to zero. That is why instead of considering more molecules in the same series, different homologous series should be introduced.

Finally, it should be noted that the data for all of the molecules were taken only from ChemSpider, as long as the circumstances didn't require otherwise. This means that the values typically weren't cross-checked with other sources and may have been inaccurate. Further studies should collect data from multiple sources and use the average values, to achieve better results.

# Works Cited

- Centers for Disease Control and Prevention (CDC). "Formamide." 11 April 2016. *The National Institute for Occupational Safety and Health (NIOSH).* Web. 13 March 2017.
  - <https://www.cdc.gov/niosh/npg/npgd0295.html>.
- ChemicalBook. "Formamide." 2016. ChemicalBook. Web. 13 March 2017.
- <a>http://www.chemicalbook.com/chemicalproductproperty\_en\_cb9854215.htm>.</a>
- Gray, Theodore. "Electronegativity of the elements." n.d. PeriodicTable.com. Web. 13 March 2017.
  - <a>http://www.periodictable.com/Properties/A/Electronegativity.al.log.html>.</a>
- Hanson, Robert. "[Jmol-users] molecular dipoles." 11 September 2014. *Jmol, Sourceforge.* Web. 13 March 2017. <a href="https://sourceforge.net/p/jmol/mailman/message/32823090/>">https://sourceforge.net/p/jmol/mailman/message/32823090/</a>.
- Molinspiration. "Molecular Polar Surface Area PSA." n.d. *Molinspiration.* Web. 13 March 2017. <a href="http://www.molinspiration.com/services/psa.html">http://www.molinspiration.com/services/psa.html</a>.
- National Institute of Standards and Technology (NIST). "Comparison of polarizabilities for LSDA/6-311G." October 2016. *Computational Chemistry Comparison and Benchmark DataBase.* Web. 13 March 2017. <a href="http://cccbdb.nist.gov/polcalccomp2.asp?method=51&basis=7">http://cccbdb.nist.gov/polcalccomp2.asp?method=51&basis=7</a>.
- National Institutes of Health (NIH). "Formamide." 12 November 2016. *PubChem.* Web. 13 March 2017. <a href="https://pubchem.ncbi.nlm.nih.gov/compound/formamide">https://pubchem.ncbi.nlm.nih.gov/compound/formamide</a>.
- Purdue University. "London Dispersion Forces." n.d. *Purdue Department of Chemistry.* Web. 13 March 2017. <a href="https://www.chem.purdue.edu/gchelp/liquids/disperse.html">https://www.chem.purdue.edu/gchelp/liquids/disperse.html</a>.
- -. "Vapor Pressure." n.d. Purdue Department of Chemistry. Web. 13 March 2017.
  <a href="https://www.chem.purdue.edu/gchelp/liquids/vpress.html">https://www.chem.purdue.edu/gchelp/liquids/vpress.html</a>.
- Royal Society of Chemistry. n.d. Chemspider. Web. 13 March 2017. < http://www.chemspider.com/>.
- University of Sydney. "Chemistry 2, Lecture 9, Raman Spectroscopy." n.d. University of Sydney, Faculty of Science. Web. 13 March 2017. <a href="https://scilearn.sydney.edu.au/fychemistry/chem2401/l9.pdf">https://scilearn.sydney.edu.au/fychemistry/chem2401/l9.pdf</a>>.
- Yamamoto, Hiroshi. "Calculation of Dipole Moment." 28 June 2011. *Pirika*. Web. 13 March 2017. <a href="https://www.pirika.com/ENG/TCPE/DP-Theory.html">https://www.pirika.com/ENG/TCPE/DP-Theory.html</a>.