How Can We Understand Molecular Bond Angles Rather Than Just Memorising Them?

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1 Introduction

Since I have an avid interest in both Chemistry and Mathematics, I wanted to explore one of the many connections they share, particularly molecular bond angles.

One of the key concepts we will be using in these derivations is 'VSEPR theory' which stands for 'Valence Shell Election Pair Repulsion theory.' Developed by Linus Pauling, this theory explains that electron orbitals (s, p, d) mix to form hybrid orbitals ($sp, sp^2\ etc$) which allow atoms to form equivalent bonds in specific directions hence why the 4 bonds in Methane (CH_4) are identical. Ronald Gillespie and Ronald Nyholm further developed this theory to predict the shapes of different molecules. Their formalised theory explains that electron pairs surrounding a central atom arrange themselves as far apart as possible, due to them having their equal charges, to minimise repulsion. As well as this they discovered that repulsion between different electron pairs (bonding and lone pairs) differs, mathematically expressed as:

$$Lone\ Pair, Lone\ Pair > Lone\ Pair, Bonding\ Pair > Bonding\ Pair, Bonding\ Pair \quad (*)$$

VSEPR theory allows us to also predict different molecular geometries, such as linear, trigonal planar, tetrahedral, trigonal bipyramidal and octahedral, this raises the question if electron pairs maximise separation, what angle can mathematics predict?

2 Derivations

2.1 Simpler Derivations of Simple Molecules

We can begin with CO_2 (Carbon Dioxide) which has 2 double bonding pairs connected to each of the Oxygen atoms and no lone pairs on the central Carbon atom. This means that the molecule will not experience any repulsion that would alter the shape of it.

Since the molecule only has 2 double bonds, from the C atom to each of the O atoms, we can deduce that this molecule lies in a single plane where all its atoms are aligned, and so we can also deduce that the bond angles for CO_2 are 180^o. This is what we call 'linear.'

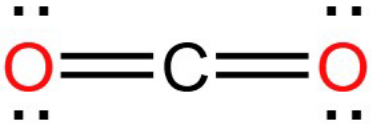


Figure 1: Lewis structure of CO_2

We can use a similar technique to derive the bond angles for a trigonal planar molecule, meaning the molecule has 3 bonds that all lie in the same plane, similarly to a linear molecule. We can take BF_3 (Boron Trifluoride) which is a trigonal planar molecule. As this molecule has 3 bonds that are separated by the maximum distance from each other due to electrostatic repulsion, we can split the angle around a point into 3 equal angles by dividing 360 by 3 – giving us 120° for each bond angle.

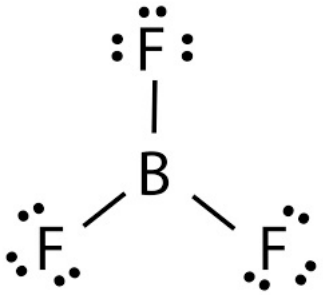


Figure 2: Structure of Boron Trifluoride

2.2 Derivation of a Tetrahedral Molecule

For example, CH_4 (Methane) is a tetrahedral molecule since it has 4 bonding pairs and no lone pairs meaning, in a 3D space, each pair is spaced equally apart. This allows us to derive the bond angle by beginning with the shape of a regular tetrahedron where the centre is at the origin (0,0,0). We can let the vertices of the shape be A(1,1,1), B(-1,-1,1), C(-1,1,-1) and D(1,-1,-1). Now to directly find an angle between each bond, we can use vectors and the dot product formula:

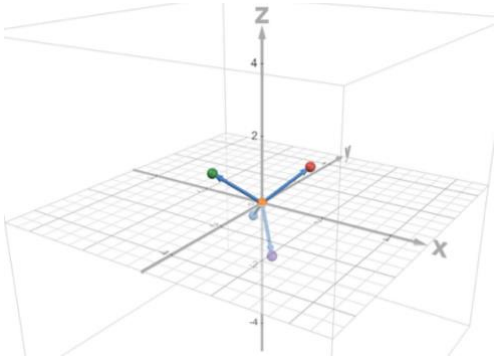
$$cos\,\theta = \frac{\boldsymbol{a}\,.\,\boldsymbol{b}}{|\boldsymbol{a}||\boldsymbol{b}|}$$

$$cos\,\theta = -\frac{1}{(\sqrt{3})(\sqrt{3})} = -\frac{1}{3}$$

$$\theta = \arccos\left(-\frac{1}{3}\right) = 109.47122\ldots^{o}$$

$$\theta \approx 109.5^{o}$$

Figure 3: Desmos 3D Representation of a Tetrahedral Molecule



This result is only possible since all electron pairs are equivalent to each other, producing a 3D symmetrical arrangement. This corresponds to the VSEPR theory where electron pairs maximise their separation in space. We can refer to this model as the 'parent arrangement' since we will be also looking at how certain molecules can deviate due to their lone pairs such as water and Ammonia (NH_3).

2.3 How and Why Molecules Deviate and Have Different Bond Angles

Molecules with at least 1 lone pair of electrons will experience electrostatic repulsion between their electron pairs due to the rule $(*)$. In the world of Chemistry, it is said that the bond angle between each pair reduces by 2.5^o due to this same rule $(*)$ so this is what we want to explain and justify. We're unable to prove this decrease of 2.5^o since I'm not quite familiar with quantum chemistry and can't solve Schrodinger's equation YET. Anyways, we can justify this claim by using Coulomb's Law where the repulsive force between regions of electron density depends on the magnitude of charge and distance between them:

$$F = \frac{kq_1q_2}{r^2}$$

We must remember that, in a bonding pair, electrons are shared between two nuclei – making the electron density spread out whereas, in a lone pair, the electron density is concentrated since the electrons are focused onto the central atom. So effectively, $q_{lone\ pair} > q_{bonding\ pair}$ by using Coulomb's Law above which reflects the inequality $(*)$. We can use a summation to show that these angles compress as there are more lone pairs:

$$E_{total} = \sum \frac{kq_1q_2}{r^2}$$

This summation can be used to explain that when lone pairs are added, the q_1q_2 terms become larger and so, to compensate, the molecule reduces particular angles to increase others where the repulsion is strongest. This effect can be seen clearly in molecules like water and Ammonia since they both have at least 1 lone pair of electrons.

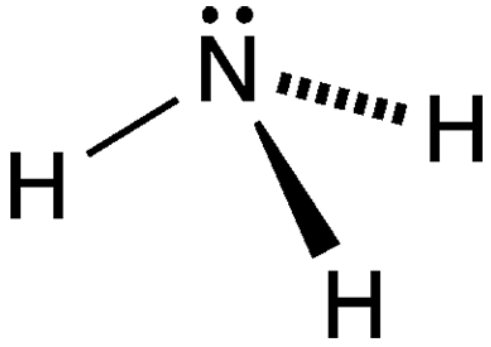


Figure 4: Structure of Ammonia

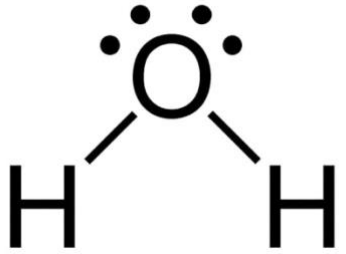


Figure 5: Structure of Water

Comparing these two molecules in Figures 4 and 5 to Methane, Ammonia and water both have lone pairs meaning their bond angles have been reduced due to the electrostatic repulsion between the lone pair(s) and the bonding pairs. Since we know that the bond angles in a molecule reduces by $2.5n$, where n is the number of lone pairs, we find that the bond angles in Ammonia are:

$$109.5 - 2.5(1) = 107^o$$

From Figure 5, we can see that water has two lone pairs and two bonding pairs. The lone pairs occupy a greater proportion of space around the central atom which causes a decrease in the bond angles so we can use the same calculation to determine the bond angle in water:

$$109.5 - 2.5(2) = 109.5 - 5$$

$$= 104.5^o$$

We treat the tetrahedral arrangement of a molecule as the 'parent arrangement' since it is the original arrangement, without any lone pairs, hence why '109.5' is used in the calculations as it is the bond angle that experiences no repulsion.

3 Conclusion

While deriving these angles, we have transitioned from simple geometric reasoning to nearly quantum wave functions. It's remarkable to see how something so simple as just angles between bonds can always be explained via mathematics without being too complex. Things like this tend to reveal how deeply mathematics governs the microscopic world.

I hope you have enjoyed the mixture of Mathematics and Chemistry while understanding the theory and concepts just like I do. Thank you for reading!