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Molecules aren't flat. They're three dimensional, and that has implications for their physical and chemical properties. For example, X-ray crystallography labs at MIT determine the 3D shapes of protein molecules to design drugs that will fit into these proteins. In this video, you'll learn about an empirical model chemists use to predict a molecule's 3D shape from its Lewis structure. This video is part of the Representations video series. Information can be represented in words, through mathematical symbols, graphically, or in 3-D models. Representations are used to develop a deeper and more flexible understanding of objects, systems, and processes. Hi. My name is Cathy Drennan and I am a professor in the chemistry department at MIT. I hope you have been enjoying your general chemistry course at SUTD. After watching this video, you will be able to use the VSEPR model to predict 3D molecular structures from 2D Lewis structures and... ...discuss some of the assumptions of the VSEPR model. Before watching this video, you should be able to draw Lewis structures for simple molecules. We can determine molecular shape experimentally or predict it with varying degrees of accuracy using empirical and theoretical models. The model that will be introduced in this video, the Valence-Shell Electron-Pair Repulsion Model, or the VSEPR model, is an empirical model, but works quite well for most simple Because it is an empirical model, the VSEPR model was constructed by looking for patterns The VSEPR model, which builds off of Lewis theory, is based on the idea that regions of high electron density repel one another. Let's take a look at the Lewis structure for NF3 to see what that means. The VSEPR model focuses on the central atoms of molecules... ...and assumes that bonding atoms... ...and lone pairs on the central atom are spaced as far apart as possible from each other to minimize electron repulsions, but at the same time are equidistant from the central atom. The VSEPR model attributes lone pairs of electrons with having a stronger repulsion than bonded electrons. And finally, the VSEPR model treats multiple bonds between 2 atoms as a single region of electron density. Let's apply the VSEPR model to a few molecules. For example, if we look at nitrous oxide, we see that there are... ...2 atoms bonded to the central atom and zero lone pairs of electrons on the central atom. To minimize electron repulsions, we will maximize the distance between the two bonded atoms by placing them along a line on either side of the central N atom. We can also see that if we placed one of the bonded atoms elsewhere, we would not have maximized the distance between the bonded atoms. We would describe nitrous oxide as having a linear geometry. In a linear molecule, the bond angle between atoms is 180 degrees. Note that when we examined the Lewis structure for nitrous oxide, the triple bonded nitrogen was treated the same as the single bonded oxygen atom. Chapter Break Now, if we followed a similar procedure for sulfur trioxide, ... we see that there are 3 atoms bonded to the central atom and zero lone pairs on the central atom. To maximize the distance of the bonding atoms from each other, we will space them 120 degrees apart around the central atom... ...on the vertices of an equilateral triangle. We would describe sulfur trioxide as a trigonal planar molecule... ...with bond angles of 120 degrees. Chapter Break Now let's take a look at SO2. Notice that you can draw resonance structures for SO2, but because VSEPR doesn't distinguish b/w single and multiple bonds, we can look at any resonance structure when predicting geometry. So let's just focus on one of these structures. What do you think the geometry of this molecule will be? Pause the video, draw a picture or construct the molecule using a molecule kit, and continue playing the video to see if you are correct. Remember, the VSEPR model assumes that bonding atoms AND lone pairs on the central atom are spaced as far apart as possible. On SO2 we have two atoms bonded to the central atom and one lone pair on the central atom. So, we have 3 regions of electron density total. Think about how you would space these 3 regions as far apart as possible. By placing them on the vertices of an equilateral triangle. On our model, this (pointing at electron cloud) represents the lone pair of electrons. While we have to think about lone pairs of electrons when predicting geometry, the naming convention actually ignores them. So, if we were to name this shape, we would focus on the shape that is determined by the atoms. We call this shape "bent". It's tempting to say that the bond angle will be 120 degrees, but bond angles in molecules with lone pairs on the central atom have been observed to be smaller than expected. One possible explanation is that a lone pair can spread over a larger region than bonded electrons causing the bonded atoms to move farther from the lone pair and closer to each other, compressing the bond angle. The VSEPR model accounts for this by saying that lone pairs repel more strongly than bonded electrons. The result is that the bond angle on sulfur dioxide will be less than 120 degrees, but VSEPR theory cannot tell us what the precise bond angle will be. Chapter Break Let's do another example - CH3Cl (chloromethane, a.k.a. methyl chloride). What do you think the geometry of this molecule will be? Pause the video, draw a picture or construct the molecule using a molecule kit, and continue playing the video to see if you are correct. How many atoms are bonded to the central atom? 4 How many lone pairs are on the central atom? 0 If we are only thinking in 2-dimensions, it's tempting to place the 4 regions of electron density at 90 degree angles to each other, ...but this would be incorrect. Remember, we're working in 3-dimensions. To maximize the distance of 4 regions of electron density, we can think about them lying at the 4 corners of a tetrahedron. It may help to review what a tetrahedron looks like. A tetrahedron is a pyramid constructed from 4 equilateral triangles. It has a triangular base and sides made from triangles. This results in 4 corners, or vertices. We imagine our central atom to be at the center of the tetrahedron. In a tetrahedral geometry, the bond angle between bonding atoms is 109.5. This is larger than the 90 degrees predicted by putting all 4 regions in the same plane The correct model of CH3Cl would look like this. This shape is aptly named a tetrahedron. Chapter Break Let's do another example -- nitrogen trifluoride. What do you think the geometry of this molecule will be? Pause the video, draw a picture or construct the molecule using a molecule kit, and continue playing the video to see if you are correct. How many atoms are bonded to the central atom? 3 How many lone pairs are on the central atom? 1 Again, we have to make sure we count the lone pair of electrons. Again, to maximize the distance of 4 regions of electron density, we can think about them lying at the 4 corners of a tetrahedron with the central atom at the center of the tetrahedron. If we build this with our kit, it looks like this. As we said earlier, the nomenclature that is used to describe molecular shapes only focuses on the positions of

As I said earlier, the nomenclature that is used to describe molecular shapes only focuses on the positions of atoms. So, if we ignore the lone pair, we're left with a shape called a trigonal pyramid. Because the trigonal pyramid is based off of the tetrahedron, we would normally predict the bond angles to be 109.5 degrees. However, the lone pair will repel the bonded electrons more strongly, causing a compression of bond angles. The bond angles in a trigonal pyramid will be less than 109.5 degrees. Chapter Break Now I encourage you to predict the geometry of sulfur hexafluoride. Pause the video, draw a picture or construct the molecule using a molecule kit, and continue playing the video to see if you are correct. How many atoms are bonded to the central atom? 6 How many lone pairs are on the central atom? 0 To maximize the distance of 6 regions of electron density, they lie at the vertices of an octahedron. Let's take a closer look at the octahedron. An octahedron is composed of 8 triangles and has 8 sides, but only 6 vertices. If we constructed sulfur hexafluoride with our kit, it would look like this. This shape is called an octahedron. The bond angle in an octahedral geometry is 90 degrees. Chapter Break Let's try one that's a little differentâ€"bromine pentafluoride. Pause the video, draw a picture or construct the molecule using a molecule kit, and continue playing the video to see if you are correct. How many atoms are bonded to the central atom? 5 How many lone pairs are on the central atom? 1 Again, to maximize the distance of 6 regions of electron density, they lie at the vertices of an octahedron. Our model would look like this. Remember, we only name geometric shapes in chemistry based on the position of atoms, so we ignore the lone pair. This shape is called a square pyramid. Because the square pyramid is based off of the octahedral geometry, we would normally predict the bond angles to be 90 degrees. However, the lone pair will repel the bonded electrons more strongly, causing a compression of bond angles. The bond angles in a square pyramid will be less than 90 degrees. Chapter break These were just a few examples to help get you started with visualizing molecules in 3D. There are other variations of these base geometries listed in your textbook that you should make sure you are familiar with. The VSEPR model is a simple, empirical model that works well for predicting the geometry of most simple molecules, but it's important to remember that as is true for all models, it is based on some assumptions that limit its range of validity. As you progress in your studies and begin to look at more complex molecules such as proteins, you will find that you will need to use more complicated models in order to generate 3D representations of these molecules. In this video, you learned that the VSEPR model can be used to help understand a simple molecule's 3D structure. In order to do this, you need to start with the Lewis structure for the molecule of interest and count how many atoms are bonded to the central atom and how many lone pairs are on the central atom. Then, you need to think about how you can position those regions as far apart from one another as possible. This is where thinking about polyhedra is useful because the vertices of polyhedra are at a maximum distance from each other. Finally, you should remember that the naming convention for molecular geometries focuses on the locations of the atoms only. Because of the simplicity of the VSEPR model, it is an easy way for you to learn how to translate 2D representation of molecules into 3D. With some practice, visualizing molecules in 3D can become second nature to you.