Color by number molecular geometry and polarity

Molecular geometry, also known as the molecular structure, is the three-dimensional structure or arrangement of atoms in a molecule. Understanding the molecular structure of a compound can help determine polarity, reactivity, phase of matter, color, magnetism, as well as biological activity. To determine the molecules' shapes, we must become acquainted with Lewis's electron dot structure. Although the Lewis theory does not determine the forms of molecules, it is the first step in predicting the forms of molecules. The Lewis structure helps us identify the bond pair and the single couple. Then, with Lewis's structure, we apply the valence-shell electron-pair repulsion (VSPER) theory to determine the molecular geometry and electron-group geometry. To identify and get a complete description of the three-dimensional shape of a molecule we need to know also learn about the state bond angle as well. Lewis Electron Dot Structures play a crucial role in determining the geometry of molecules because it helps us identify the valence electrons. To learn how to draw a Lewis electron dot structure click on the link above. Now that we have a background in lewis electron dot structure, we can use it to find the valence electrons of the center atom. Valence-shell electron-pair repulsion (VSEPR) theory that electron pairs repel each other, whether they are in bond pairs or in single pairs. Thus, electron pairs will spread as far apart as possible to minimize repulsion. VSEPR focuses not only on electron pairs, but also focuses on electron groups as a whole. An electron group can be an electron pair, a lone pair, a single lone electron, a double binding or a triple binding on the center atom. Using the VSEPR theory, electron bond pairs and single pairs at the center atom will help us predict the shape of a molecule. The shape of a molecule is determined by the position of the nuclei and its electrons. The electrons and nuclei sit down in positions that minimize repulsion and maximize attraction. Thus, the shape of the molecule reflects its equilibrium state, where it has the lowest possible energy in the system. Although VSEPR theory predicts the distribution of electrons, we have to take into account the actual determinant of the molecular form. We distinguish this into two categories, electron-group geometry and molecular geometry. Electron group geometry is determined by the number of electron groups. Number of electron groups Name of electron group geometry 2 linear 3 trigonal-planar 4 tetrahedral 5 trigonal bipyramidal 6 octahedral Molecular geometry depends not only on the number of electron groups, but also on the number of single pairs. When the electron groups are all pairs of binders, they are named exactly as the geometry of the electron group. See chart below for information on how they are named depending on the number of single pairs the molecule has. As mentioned above, molecular geometry and electron group geometry are the same when there are no single pairs. The VSEPR listing for these molecules is AXn. A represents the central atom and n represents the number of bonds with the central atom. When single pairs are present, the letter Ex. X represents the number of single pairs present in the molecule. For example, a molecule with two pairs of binding pairs and two single pairs would have this notation: AX2E2. Geometry of molecules Diagram Number of electron groups Electron group Geometry Number of single pairs VSEPR Notation Molecular Geometry Ideal Bond Angles Examples 2 linear 1 AX2 180° BeH2 3 trigonal planar 0 AX3 120° CO32- 1 AX2E

120° O_3 4 tetraralt 0 AX_4 Tetrahedral 109.5° SO_4^{2-} 1 AX_3E 109.5° H_3O^+ 2 AX_2E_2 109.5° H_2O 5 trigonal bee Pyramidal 0 AX_5 90°, 120° PF_5 1 AX_4Eb 90° 120° $TeCl_4$ 2 AX_3E_2 90° ClF_3 3 AX_2E_3 180° I_3-6 Octane 0 AX_6 octaveral 90° PF_6^-1 AX_5E 90° $SbCl_5^{2-}$2 AX_4E_2 90° ICl_4^- Example \(\PageIndex{1}\): Let's try to determine the geometric structures of H_2O and CO_2. So start by drawing Lewis's structure: H_2O: Water has four electron groups, so it falls under the tetrahedral for electron-group geometry. The four electron groups are the 2 single bonds for Hydrogen and the 2 single pairs of oxygen. Since water has two single pairs, the molecular shape is bent. According to VSEPR theory, the electrons want to minimize repulsion, thus as a result, the single pairs adjacent to each other. CO_2: Carbon dioxide has two electron groups and no single pair. Carbon dioxide is therefore linear in electron group geometry and in molecular geometry. The shape of CO_2 is linear because there are no single pairs that affect the direction of the molecule. Therefore, linear orientation minimizes repulsion forces. The VSEPR theory not only applies to a central atom, but also applies to molecules with more than one central atom. We take into account the geometric distribution of the terminal atoms around each central atom. For the final description, we combine the separate description of each atom. In other words, we take long-chain molecules and break them down. Each piece will form a specific shape. Follow the example below: Butane is C_4H_{10}. C-C-C is the simplified structural formula in which the hydrogen (not shown) is understood to have individual bonds to Carbon. You can see a better structural formula of butane on en.Wikipedia.org/wiki/File:Butane-2D-flat.png If we break down each Carbon, the central atoms, into pieces, we can determine the relative shape of each section. Let's start with the left side. We can see that C has three single bindings for 2 hydrogens and a single bond for Carbon. This means that we have 4 electron groups. By controlling the geometry of molecules above we have a tetrahedral shape. Now we move on to the next Carbon. This Carbon has 2 single bonds for 2 Carbons and 2 single bonds for 2 Hydrogens. Again we have 4 electron groups which result in a tetrahedral. Continuing this trend, we have another tetrahedral with single bonds attached to hydrogen and carbon atoms. As for the rightmost Carbon, we also have a tetrahedral where Carbon binds with a Carbon and 3 Hydrogens. Let me recap. We took a look at the butane provided by the wonderful Wikipedia link. We broke the molecule in parts. We did this by looking at a particular central atom. In this case, we have 4 central atoms, all Carbon. By breaking the molecule into 4 parts (each part looks at 1 of the 4 carbons), we determine how many electron groups there are and find out the shapes. We're not done yet! We have to determine if there are any single couples because we only looked at bonds. Remember that electron groups include single couples! Butane has no single couple. Therefore, we have 4 tetrahedrals. What should we do with 4 tetrahedrals? We will optimize the binding angle for each central atom attached to each other. This is because the electrons shared are more likely to reject each other. With 4 tetrahedrals, the shape of the molecule looks like this: en.Wikipedia.org/wiki/File:Butane-3D-balls.png. This means that if we look back at each single tetrahedral, we match the central carbon with the Carbon it is bound to. Bond angles also contribute to the shape of a molecule. Bond angles are the angles between adjacent lines representing bonds. The binding angle can help distinguish between linear, trigonal planar, tetraheral, trigonal-bipyramidal, and octahedral. The ideal binding angles are the angles that show the maximum angle at which it would minimize repulsion, thus controlling vsepr theory. Essentially, bond angles tell us that electrons don't like being near each other. Electrons are negative. Two negatives don't attract. Let's create an analogy. In general, a negative person is seen as bad or mean and you don't want to talk to a negative person. A negative person is bad enough, but if you have two put together... It's just horrible. The two negative people will be mean to each other and they won't like each other. So they will be far away from each other. We can apply this idea to electrons. Electrons are similar in charge and will reject each other. The furthest way they can get away from each other is through angles. Let's refer to tetrahedrals. Why is it that 90 degrees doesn't work? If we pull out a tetrahedral on a 2D plane, we'll get 90 degrees. But we live in a 3D world. If you want to visualize this, think about movies. Movies in 3D pop out at us. Before, we're watching movies that are right on screen, and that's good. What's better? or 2D? For binding angles, 3D 3D Therefore, tetrahedrals have a bond angle of 109.5 degrees. How the researchers got this number was through experimentation, but we don't need to know too much detail because it is not described in the textbook or lecture. Using the example above, we would add that H_2O has a binding angle of 109.5°, and CO_2 would have a binding angle of 180°. To summarize there are four simple steps to apply VSEPR theory. Draw the Lewis structure. Count the number of electron groups and identify them as connecting pairs of electron groups or single pairs of electrons. Remember electron groups include not only bonds, but also single couples! Name of the electron group geometry. (State whether it is linear, trigonal-planar, tetrahedral, trigonal-bipyramidal, or octahedral.) Looking at the location of other atomic nuclei around the central determine molecular geometry. (See how many single couples there are.) A molecule is polar when the electrons are not distributed equally and the molecule has two poles. The more electronegative end of the molecule is the negative end, and the less electronegative end is the positive end. A common example is HCl. Use of capital sigma + or - as a symbol to show the positive end and the negative end we can withdraw the net dipole. So sigma + would be on hydrogen atom and sigma - would be on chlorine atom. Using the cross bow arrow shown below we can show that it has a net dipole. The net dipole is the measurable, called dipole-eye mode. Dipole moment is equal to the product of the partial charge and the distance. The equation for dipol moment is as follows. $$\mu = \delta \times d$$ with μ = dipole torque (debye) δ = partial charging (C) d = distance (m) The units of dipole expressed in the bye, which is also known as Coulombs x meter (C x m) Example of a Dipole Cross arrow shows the net dipole. On the cross-bottomer, the cross represents the positive charge, and the arrow represents the negative charge. Here's another way to determine dipol moments. We need to understand electronegativity which is abbreviated EN. What is EN? Well, one is how much an element really wants an electron. Think about basketball and how two players pass the ball on to each other. Each player represents an element, and the ball represents the electron. Let's say a player is a ball game. The player who is ball hog is more electronegative because he or she wants the ball more. Here is a link that has all the EN listed: www.green-planet-solar-energy ... Electroneg.gif What if we don't get EN? Fortunately, there is a trend in the periodic table for EN. From bottom to top, EN will increase. From left to right, EN will rise. The most electronegative element is Flourine with 4.0. Now we are ready to use EN to determine whether molecules are polar or not. We look back at the picture of H_2O above. ONE is given. What do we do with all the We compare ONE between each bond. Oxygen has a larger EN than Hydrogen. That's why we can draw a cross bow arrow against Oxygen. We have two arrows because Oxygen is bound to two hydrogens. Since both arrows point towards Oxygen, we can say that there is a net EN. We've added the arrows pointing to Oxygen, and we're going to end up with a new, bigger arrow. This is examplified in the image above. If arrows are pulled away from each other like <--- and --->, then we are more likely to have something net EN because the molecule is symmetrical. Look back to the Lewis dot chart of CO_2. The shape is linear and the EN arrows point to oxygen. The arrows are opposite to each other and have the same EN difference. Therefore, we have no net charge, and the molecule is non-polar. To summarize, when a molecule is polar, this means that the electron is not distributed evenly, and there is a difference in the electron ability of the atoms. If a molecule is polar, it means it had a net dipole, resulting in having a dipole moment. Is it polar? There are three ways to go about determining whether a molecule is polar or not. If the molecule has a net dipole, then it's polar. B. If the structure is symmetrical, then it is non-polar C. There are three rules for this part: 1. When there are no single pairs on the middle atom, then the molecule is non-polar 2. If it is linear or square planar, then it is non-polar. (This rule is more important than Rule 1, so it overrides it because it has single pairs.) 3. If it has different terminal atoms, then it is polar. (This rule overrides rules 1 and 2 because it is more important.) Petrucci, Ralph H., William S. Harwood, F. Geoffrey Herring, & Jeffry D. Madura, General Chemistry, Principles and Modern Appplications Ninth Edition, Upper Saddle River, New Jersey Tetrahedrality and the relationship between collective structure and radial distribution functions in liquid water P. E. Mason and J. W. Brady J. Phys. Chem.B;2007 Inverted geometries on carbon Kenneth B. Wiberg Acc. 1984 Molecular geometries. Chemistry funds and applications. Volume 3. Farmington, MI:Lagowski, J.J., 2004. Draw Lewis's structure and name the shape of each substance. Also determine polarity and whether it has a dipole moment. $HClO_3$ SO_3 PCl_4 C_2H_4 $SnCl_3^-$ Name yeast shape and determine if they are polar or non-polar. 1. Total # of electrons: 1 +(3x6)+7=26 electron group geometry: tetrahedral molecular: trigonal pyramideal ideal angle: 109.5 ° polar, has a dipole moment 2. Total number of electrons: (3x6)+6=24 electronic group geometry: trigonal planar molecular geometry: trigonal planar ideal angle: 120° polar, has a dipole eye torque 3. Total number of electrons: (4x4)+5=5=19 electronic group geometry: trigonal-bi-pyramidal molecular geometry: tilt ideal angle: 90°, 120° polar, has a dipole eye-up 4. Total electrons: (1x4)+(4x2)=12 group geometry: trigonal planar molecular geometry: trigonal planar ideal angle: 120° non-polar, does not have a dipole moment 5. Total number of electrons: (7x3)+4=26 electronic group geometry: tetrahedral molecular geometry: trigonal pyramideal ideal angle: 109.5° polar, has a dipole eye mode. 1. electron group geometry: octahedral molecular geometry: square planar not polar because it is symmetrical 2. electron group geometry: octahedral molecular geometry: square planar polar, because it is not symmetrical symmetrical symmetrical