Molecular Geometry and Dipole Moments

Lewis Dot Structures->VSEPR->Molecular Geometry->Dipole Moment

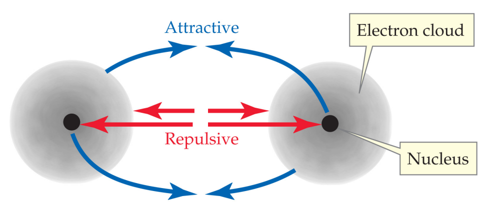
Today's Lecture

- Review sigma and pi pond, and how they relate do single, double and triple bonds
- Revisit Lewis Dot Structures
- Use Lewis Dot Structures to Predict Molecular Geometry (VSEPR)
- Molecular Geometry and Dipole Moments
- Molecular Ions

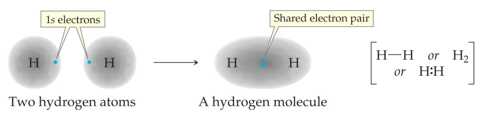
Covalent Bonds

- These bonds are formed when atoms share electrons.
- The electrons are shared in such a way that each atom gets all it needs. (Imagine a system in which when we share a cookie we each get a whole one.)
- This sharing can occur when electrons are located mostly between the atoms (sigma bonds) or above and below the atoms (pi bonds)

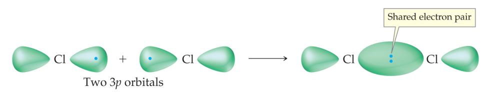
When the nucleus–electron attractions (blue arrows) are greater than the nucleus–nucleus and electron–electron repulsions (red arrows), the result is a net attractive force that holds the atoms together to form a molecule.



- Covalent bond formation in H_2 can be visualized by imagining that the two spherical 1*s* atomic orbitals blend together and overlap to give an egg-shaped molecular orbital.
- Both atoms share the two valence electrons and the stability of the closed shell electron configuration.
- This bond is a **sigma** bond that is made with two 1s orbitals.

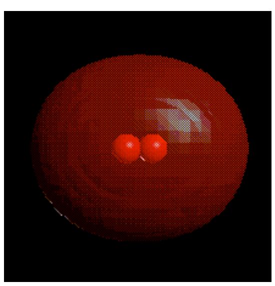


- Bond formation in Cl_2 also can be pictured as the overlap of the two 3p atomic orbitals.
- The molecular orbital formed creates a region of high electron density between the two nuclei.
- In this bond the electron density is greatest between the atoms. The bond is a **sigma** bond made using a 3p orbital from each atom.



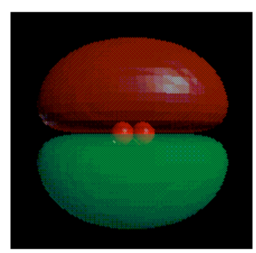
O_2 – Sigma Bond (σ bond)

- Oxygen atoms interact to form molecular oxygen, O_2.
- In O_2there is one orbital formed using valence electrons that increases the electron density between the oxygen atoms. It has a sphere-like shape.
- This is a sigma bond.



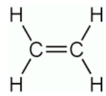
O_2 – Pi Bond (π bond)

- When the oxygen atoms interact an additional bond is formed. This is formed when p orbitals on the 2 atoms overlap.
- This is a pi bond.
- The electron density is concentrated above and below the joined atoms.



Returning to the Video

- Animation of the formation of ethylene.

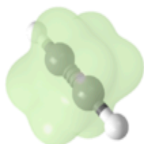


- http://www.youtube.com/watch?v=C2W-yDPcpl4
- The 3 orbitals on each carbon shift to form 3 new orbitals. Of these 2 are used to make a sigma bond. The unchanged p orbitals overlap to form the pi bond.

Triple Bonds - Acetylene

- Sometimes 2 sets of p orbitals overlap to form pi bonds. This is in addition to the sigma bond. When this happens a triple bond is formed.

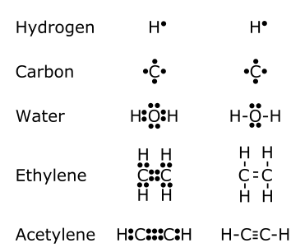
http://andromeda.rutgers.edu/~huskey/images/acetylene_bonds.jpg



Lewis Dot Structures

- Dot Structures are diagrams that contain symbols of elements as well as dots.
- The symbols represent atoms in molecules and the dots represent valence electrons.
- The dots are a way to keep track of electrons.
- This structure allow us possible predict the number bonds between atoms in molecules, and the number electrons that are not part of these bonds. (We do this with out explicit use of quantum mechanics or sophisticated consideration of molecular orbitals.)

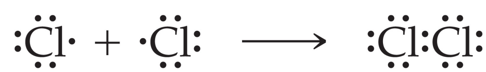
- These diagrams show bonding electrons between the element symbols, and nonbonding electrons. The nonbonding electros are pairs of located on the sides of the symbol.



Lewis Structures-Things to Remember

- Only the valence electrons appear in a Lewis structure.
- Bonds are made in order to fill the outer shell of the element.
- Bonds are indicated by electron pairs shown between the element symbols.
- There may be as many as three bonds between a pair of atoms.
- Stable molecules will only have paired electrons.
- These are only useful cartoons.

- An individual Cl atom has 7 valence electrons. 6 of these are paired and the 7th is unpaired.
- When two Cl atoms approach each other, the unpaired 3p electrons are shared by both atoms in a covalent bond.
- Each Cl atom in the molecule now “owns” six outer-shell electrons and “shares” two more, giving each a valence shell octet like that of the noble gas Ar.



Should we do an example or two

- CH_3Cl
- O_3
- CH_2O

Predicting Geometry-VSEPR

The *V*alence *S*hell *E*lectron *P*air *R*epulsion (VSEPR) model:

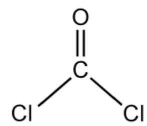
- is based on the number of regions of high electron density around a central atom.
- can be used to predict structures of molecules or ions that contain only non-metals by minimizing the electrostatic repulsion between the regions of high electron density.
- can also be used to predict structures of molecules or ions that contain multiple bonds or unpaired electrons.
- does fail in some cases.

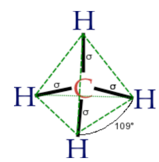
To Use Vesper

1 Draw Lewis Structure
2 Count the number of objects around the central atom (electron pairs and atoms)
3 Determine the shape formed by all of the objects
4 Disregard the electrons but keep the shape the same.

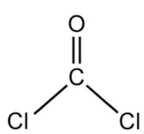
The VSEPR model uses that fact that electron clouds will repel one another, and so keep as far apart as possible.

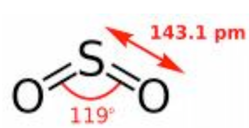
- If there are 2 objects the objects will be arranged in a line.
- If there are 3 objects it will be trigonal planar.
- If there are 4 objects they will form a tetrahedron





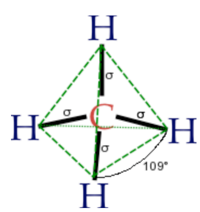
Trigonal Planar

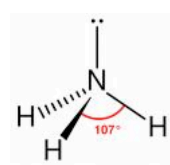




Sulfur dioxide (SO2) has an unpaired electron on the sulfur. There are 3 objects around the central atom, just as there are carbonyl dichloride (Phosgene).

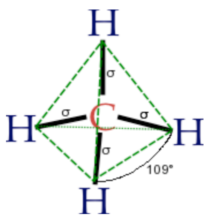
Tetrahedral

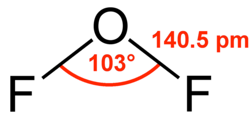




- Methane is tetrahedral but with the same number of objects ammonia is pyramid.

Tetrahedral



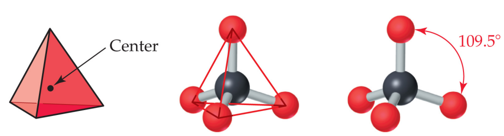


- Methane has 4 objects and so is a tetrahedral shape, water ha bent shape with an anlge close to that seen in the tetrahedron.

TABLE 5.1 Molecular Geometry Around Atoms with 2, 3, and 4 Charge Clouds

NUMBER OF BONDS	NUMBER OF LONE PAIRS	NUMBER OF CHARGE CLOUDS	MOLECULAR GEOMETRY	EXAMPLE
2	0	2	Linear	$O{=}C{=}O$
3	0	3	Planar triangular	$H_2C{=}O$
2	1		Bent	O_2S
4	0	4	Tetrahedral	CH_4
3	1		Pyramidal	NH_3
2	2		Bent	H_2O

- Linear molecules have bond angles of 180°.
- Planar triangular molecules have bond angles of 120°.
- Tetrahedral molecules have bond angles of 109.5°.

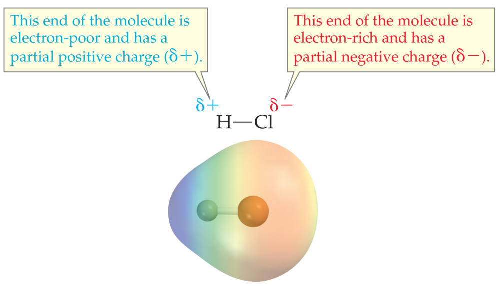


A regular tetrahedron (a) (b) A tetrahedral molecule (c)

5.8 Polar Covalent Bonds and Electronegativity

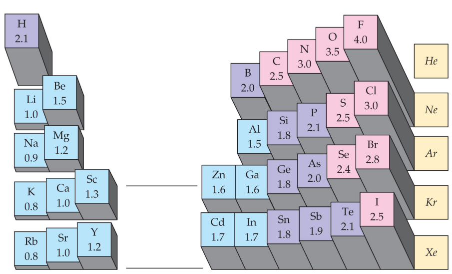
- Electrons in a covalent bond occupy the region between the bonded atoms.
- If the atoms are identical, as in H_2 and Cl_2, electrons are attracted equally to both atoms and are shared equally.
- If the atoms are not identical, however, as in HCl, the bonding electrons may be attracted more strongly by one atom than by the other and thus shared unequally. Such bonds are known as **polar covalent bonds**.

When charges separate in a neutral molecule, the molecule has a dipole moment and is said to be polar.

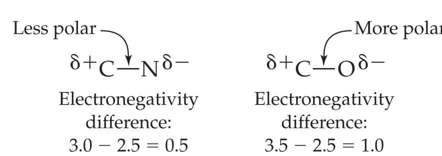


- In HCl, electrons spend more time near the chlorine than the hydrogen. Although the molecule is overall neutral, the chlorine is more negative than the hydrogen, resulting in partial charges on the atoms.
- Partial charges are represented by a δ- on the more negative atom and δ+ on the more positive atom.
- The ability of an atom to attract electrons is called the atom's **electronegativity**.
- Fluorine, the most electronegative element, assigned a value of 4, and less electronegative atoms assigned lower values.

Elements at the top right of the periodic table are most electronegative, those at the lower left are least electronegative. Noble gases are not assigned values.



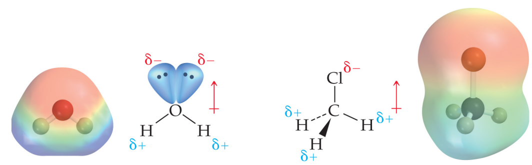
- As a rule of thumb, electronegativity differences of less than 0.5 result in nonpolar covalent bonds, differences up to 1.9 indicate increasingly polar covalent bonds, and differences of 2 or more indicate ionic bonds.
- There is no sharp dividing line between covalent and ionic bonds; most bonds fall somewhere in-between.



5.9 Polar Molecules

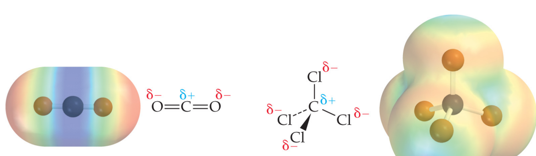
- Entire molecules can be polar if electrons are attracted more strongly to one part of the molecule than to another.
- Molecules polarity is due to the sum of all individual bond polarities and lone-pair contribution in the molecule.
- Polarity has a dramatic effect on the physical properties of molecules, particularly on melting points, boiling points, and solubility.

- Dipoles or polarity can be represented by an arrow pointing to the negative end of the molecule with a cross at the positive end resembling a + sign.



Water, H_2O Chloromethane, CH_3Cl

- Just because a molecule has polar covalent bonds does not mean that the molecule is polar overall.
- Carbon dioxide and tetrachloromethane molecules have no net polarity because their symmetrical shapes cause the individual bond polarities to cancel each other out.



Zero net polarity Zero net polarity

Molecular Ions

- Often a molecule can take on a charge.
- When this happens it is usually because there is some reason that the electron configuration is more stable with an extra electron or two, or because it is more stable without these electrons.
- Molecular ions are also called polyatomic ions.

4.9 Polyatomic Ions

- Ions that are composed of more than one atom are called **polyatomic ions**.
- Most polyatomic ions contain oxygen and another element, and their chemical formulas show by subscripts how many of each type of atom are combined.
- Sulfate ion, for example, is composed of one sulfur atom and four oxygen atoms, and has a charge of -2; the entire group of atoms acts as a single unit.

TABLE 4.4 Some Common Polyatomic Ions

NAME	FORMULA	NAME	FORMULA
Hydronium ion	H_3O^+	Nitrate ion	NO_3^-
Ammonium ion	NH_4^+	Nitrite ion	NO_2^-
Acetate ion	$CH_3CO_2^-$	Permanganate ion	MnO_4^-
Carbonate ion	CO_3^{2-}	Phosphate ion	PO_4^{3-}
Hydrogen carbonate ion (bicarbonate ion)	HCO_3^-	Hydrogen phosphate ion	HPO_4^{2-}
		Dihydrogen phosphate ion	$H_2PO_4^-$
Dichromate ion	$Cr_2O_7^{2-}$	Sulfate ion	SO_4^{2-}
Cyanide ion	CN^-		
Hydroxide ion	OH^-	Hydrogen sulfate ion (bisulfate ion)	HSO_4^-
Hypochlorite ion	OCl^-	Sulfite ion	SO_3^{2-}

Polyatomic Anions-The ones you need to know

- Carbonate CO^{3-}
- Sulfate SO_4^{2-}
- Hydroxide OH^-
- Nitrate NO_3^-
- Phosphate $PO_4$3-
- Acetate $CH_3CO_2^-$
- Amonium NH_4^+

- When you are making a Lewis Stucture of a polyatiomic anion just add the additional electron wherever you find that you need it at the end.
- For ammonium, the one cation on the list, just start out with 1 less.

Formulas of Ionic Compounds Containing Polyatomic Ions

- A chemical formula shows the simplest ratio of anions and cations required for a total charge of zero, just as before.
- Often the polyatomic ion is shown in parentheses. This is always done if there are more than 1 of this ion, or a combination of several polyatomic ions.

KNO_3	$Mg(NO_3)_2$	NH_4NO_3
potassium nitrate	magnesium nitrate	ammonium nitrate

Just as a reminder

- List the cation first and the anion second; for example, NaCl not ClNa.
- Make sure to eliminate any common factors from the subscripts; for example, MgO not Mg_2O_2.
- Do not write the charges of the ions; for example, KF not K^+F^-
- Use parentheses around a polyatomic ion formula if it has a subscript; for example, $Al_2(SO_4)_3$ not Al_2SO_{43}.

4.11 Naming Ionic Compounds

- Some metals form more than one ion. We need to specify the charge on the cation in these compounds. The old and new ways to do this are shown in the examples below:
- $SnCl_2$ - Tin (II) chloride
- $SnCl_4$ - Tin (IV) chloride
- $FeSO_4$ - Iron(II) sulfate

OK how about trying a few. What is the name and the formula of these?

- Cs + SO_4^{2-}
- Cr(III) + SO_4^{2-}
- Na + CO_3^{2-}
- Na + HCO_3^-
- Bicarbonate HCO_3^-

Lecture Summary

- Electron dot structures can be used to determine the types of bonds between atoms in molecules, and to predict the geometric shape of a molecule.
- Polyatomic anions can be treated with Lewis Dot structures as well.
- (Naming of polyatomic cations)