#### Chemical Bonding and Structure

Ms. Peace

#### Lesson 1

4.1 Ionic Bonding and Structure





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# Ionic Bonding

- An ionic bond is:
  - The electrostatic attraction between two oppositely charged ions
- At normal conditions they are solids with lattice structures



Ionically bonded compounds are often referred to as salts

#### Lattice Structures

- Electrostatic attraction: positive charges and negative charges attract each other
- The ions take on a predictable three-dimensional crystalline structure known as the ionic lattice
- Each sodium ion is surrounded by six chloride ions
- Each chloride ion is surrounded by six sodium ions

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# Ionic Bonding

- Electrons are gained or lost to make an ion that is isoelectronic to the nearest noble gas
  - Mg<sup>2+</sup> ion is isoelectronic with the noble gas atom neon
  - O<sup>2-</sup> ion is isoelectronic with the noble as atom neon
- The driving force for electron transfer is usually the formation of a noble gas configuration
- Transition metals can form more than one ion so they do not have noble gas electron configurations.

## Formation of Simple Ions

- Positive ions (cations) are formed when metals lose their outer shell electrons
  - ► Group 1: Li  $\rightarrow$  Li<sup>+</sup> + e<sup>-</sup>
  - ► Group 2: Ca  $\rightarrow$  Ca<sup>2+</sup> + 2e<sup>-</sup>
  - ► Group 3: Al  $\rightarrow$  Al<sup>3+</sup> + 3e<sup>-</sup>
  - Transition metals form multiple different ions
    - ►  $Fe \rightarrow Fe^{2+} + 2e^{-}$
    - ►  $Fe \rightarrow Fe^{3+} + 3e^{-}$
- Negative ions (anions) are formed when non-metals gain enough electrons to complete their outer shells
  - Group 5: N +  $3e^- \rightarrow N^{3-}$
  - Group 6: O +  $2e^- \rightarrow O^{2-}$
  - ► Group 7: F + e-  $\rightarrow$  F<sup>-</sup>

### Polyatomic Ions

- Many ions are made of multiple atoms with an overall negative charge
- The negative ones are mostly acids that have lost their hydrogens

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You need to know about:

- ► Sulfate, SO<sub>4</sub><sup>2-</sup>
- Phosphate,  $PO_4^{3-}$
- Nitrate, NO<sub>3</sub><sup>-</sup>
- ► Carbonate, CO<sub>3</sub><sup>2-</sup>

- Hydrogen carbonate, HCO<sub>3</sub><sup>-</sup>
- ► Hydroxide, OH<sup>-</sup>
- ► Ammonium, NH<sub>4</sub><sup>+</sup>

### You must know these!

Polyatomic ion name	Charge on ion	Symbol	Example of compound containing this ion
nitrate	1–	NO <sub>3</sub> -	lead nitrate
hydroxide	1-	OH-	barium hydroxide
hydrogencarbonate	1–	HCO <sub>3</sub> -	potassium hydrogencarbonate
carbonate	2–	CO32-	magnesium carbonate
sulfate	2–	SO4 <sup>2-</sup>	copper sulfate
phosphate	3–	PO4 <sup>3-</sup>	calcium phosphate
ammonium	1+	NH4 <sup>+</sup>	ammonium chloride

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## The Octet Rule

Elements tend to lose electrons, gain electrons, or share electrons in order to acquire a noble gas electron configuration.

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- Lose electrons-undergo oxidation
- Gain electrons-undergo reduction
- There are some exceptions to this rule



# Formulas of Ionic Compounds

1. Check the periodic table for the ions that each element will form. Al is in group 3, Oxygen is in group 6

2. Write the number of the charge above the ion.

3+ 2-

Al O

3. "Criss cross" the numbers to balance the charges.



4. Write the final formula using subscripts to show the number of each ion.

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 $Al_2O_3$ 

## Naming Ionic Compounds

#### The cation gives the first part of the name

- Normally a metal except in the case of ammonium  $(NH_4^+)$
- In the case of transition metals, Roman numerals tell you the charge on the metal ion
- The anion gives the second part of the name
  - Simple ions: '-ide'...e.g. chloride, fluoride, nitride etc
  - Complex ions: just their name: sulfate, phosphate etc
    - Note: the '-ate' ending usually refers to polyatomic ions containing oxygen, which provides the negativity...more on this in the redox unit
- Examples:
  - $CaF_2$ : calcium fluoride
  - Fe<sub>3</sub>(PO<sub>4</sub>)<sub>2</sub>: iron (II) phosphate

# Physical Properties of Ionic Compounds

- High melting and boiling points due to strong electrostatic forces between oppositely charged ions
  - MgO, the two charges correspond to +2 and -2 have a higher melting point than NaCl whose two charges correspond to +1 and -1
- Low volatility, how readily a substance evaporates, due to electrostatic forces of attraction
- Do not conduct electricity when solid due to fixed positions of ions, but when melted (molten) the ions are able to move around
- Aqueous solutions conduct electricity

# Physical Properties of Ionic Compounds

#### Soluble in water

#### Not usually soluble in non-polar solvents

- Solubility is determined by the degree to which the two substances mixing are attracted to each other ("like dissolves like")
- Ionic compounds can dissolve in polar substances because the positively and negatively charged ions are attracted to the partially positive and negative regions in the polar covalent compound

#### Utilization

Ionic liquids are efficient solvents and electrolytes used in electric power sources and green industrial processes



#### Lesson 2

4.2 Covalent Bonding





# **Covalent Bonding**

 A covalent bond is the attraction of two atoms to a shared pair of electrons

water Each O has two single bonds **carbon dioxide** each C has two double bonds





- Atoms aim for complete outer-shells, and each covalent bonds gives them one electron
  - Atoms form as many bonds as they have gaps in their outer-shells

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Covalent bonds typically form between two non-metals

# How many bonds?

- Atoms (usually) form bonds according to the 'octet' rule
  - This means they try to get a full outer shell of 8 electrons (except hydrogen which is full at 2)
- Atoms form as many bonds as they have 'gaps' in their outer shells, with each bond gaining them one electron:
  - Group 7: 7 electrons, 1 gap  $\rightarrow$  1 bond
  - Group 6: 6 electrons, 2 gaps  $\rightarrow$  2 bonds
  - Group 5: 5 electrons, 3 gaps  $\rightarrow$  3 bonds
  - Group 0/8: 8 electrons, 0 gaps  $\rightarrow$  0 bonds
- Covalent bonds can be:
  - Single: one shared electron pair, X-X
  - Double: two shared electron pairs, X=X
  - ► Triple: three shared electron pairs, X≡X



- Cl has 7 valence electrons
- This covalent bond is a single bond represented by a line
- There a total of 6 non-bonding pairs of electrons or lone pairs
- One bonding pair of electrons



- O has 6 valence electrons
- This covalent bond is a double bond represented by two lines
- There a total of 4 non-bonding pairs of electrons or lone pairs
   Two bonding pairs of
  - electrons



- N has 5 valence electrons
- This covalent bond is a triple bond represented by three lines
- There a total of 2 non-bonding pairs of electrons or lone pairs
- Three bonding pairs of electrons



- H has 1 valence electron
- F has 7 valence electrons
- This covalent bond is a single bond represented by a line
- There a total of 3 non-bonding pairs of electrons or lone pairs
- One bonding pair of electrons



#### Bond Strength and Length

#### Increasing strength

Single bond	Double bond	Triple bond
H-H	0=0	$N \equiv N$
H:H	0::0	N₩N

Increasing length

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## Ionic vs Covalent Bonds

Ionic Bonding	Covalent Bonding
Metal and Non-metal	Non-metal and non-metal
Atoms gain or lose electrons	Atoms share electrons
Electrostatic attraction between oppositely charged ions	Electrostatic attraction between a shared pair of electrons
Lattice structures	Consists of molecules
Higher melting and boiling points	Lower melting and boiling points
Low volatilities	May be volatile
Soluble in water	Insoluble in water
Conduct electricity when molten due to free moving ions	Do not conduct electricity because there are no ions present

## Polar Covalent Bond

- Bonding electrons shared unequally between two atoms
- One atom adopts a partial negative charge, □<sup>-</sup>, and one atom adopts a partial positive charge, □<sup>+</sup>
- Dipole moment occurs, separation of the charges, µ



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### Non-Polar Covalent Bond

- Two atoms involved in the formation of the covalent bond are identical
- There is no dipole moment



#### Dipole Moment

#### The separation of charge



molecular dipole moment







# Pauling Scale

Relative attraction that an atom has for the shared pair of electrons in a covalent bond.



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#### Electronegativity and Polarity

Bond type	Electronegativity Difference, <b>Δ</b> Χ <sub>p</sub>
lonic	ΔX <sub>p</sub> > 1.8
Non-polar Covalent	$\Delta X_p = O$
Polar Covalent	O < ΔX <sub>p</sub> ≤ 1.8

## Problems to try

Label each element as partially positive or partially positive with dipole symbols. Determine if the molecule is polar or nonpolar.

For each pair of bonds, determine which one is more polar

1. 
$$H - P$$
 or  $H - C$   
2.  $O - F$  or  $O - I$   
3.  $N - O$  or  $S - O$   
4.  $N - H$  or  $S - H$ 

- 1. **H**——Cl
- 2. **H**—–**H**
- 3. **H**—–I
- 4. Br—Br

5. C = O

#### Lesson 3

4.3 Covalent Structures





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Lewis (Electron Dot) Structures

Lewis symbols show the number of valence electrons of an element represented by dots



Lewis (electron dot) structures show bonding pairs of electrons as single, double, or triple bonds and non-bonding pairs of electrons or lone pairs, electrons not involved in the bonding in covalent molecules

### Drawing Lewis (Electron Dot) Structures

- If carbon is present, it is the backbone.
- If carbon is not present choose the least electronegative element unless the least electronegative element is hydrogen.
  - HYDROGEN WILL NEVER BE THE BACKBONE.
- All atoms should be connected to the backbone with bonds represented by a line. These lines represent bonding pairs of electrons
- Add unshared pairs of electrons (dots) to each atom so that there is an octet around each atom that maintains an octet. HYDROGEN NEVER MAINTAINS AN OCTET.The maximum number of electrons that can be shared by hydrogen is 1

## Drawing Lewis (Electron Dot) Structures

- Determine the elements present in the molecule
  CCl<sub>4</sub>
- Count the number of electrons present
  - ► 1Cx4=4
  - ▶ 4 Cl x 7 = 28
  - 32 total electrons
- Make carbon or the least electronegative element the center. HYDROGEN CAN NEVER BE THE CENTER.

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Hydrogen can only form one bond
## Drawing Lewis (Electron Dot) Structures

Draw the valence electrons around each element



## Drawing Lewis (Electron Dot) Structures

Connect the bonding pairs by connecting with a line



## Drawing Lewis (Electron Dot) Structures

Count to ensure all 32 electrons are present



## Problems to Try

- BF<sub>3</sub>
  SO<sub>2</sub>
  PH<sub>3</sub>
  NH<sub>3</sub>
- 3. CO 3. H<sub>2</sub>O

### Octet Rule

We are all familiar with the octet rule

Some atoms like B and Be might form stable compounds with incomplete octets of electrons



The expanded octet

- In this example, the Lewis structure of SO<sub>3</sub> shows it with 12 electrons in the outer shell
- This is because sulfur can make use of its empty d-orbitals (the 3d ones)
- This is called an expanded octet
  - Period 2 elements can't do this as they have no d-orbitals

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## Cations and Anions

The Lewis structure of anions and cations have brackets around them to represent a charge to the whole compound





- Valence Shell Electron Pair Repulsion theory can be used to deduce the shapes of covalent molecules
- Pairs of electrons around an atom repel each other this determines a molecule's shape
- Pairs of electrons are known as 'electron domain' and include both:

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- The electrons in a covalent bond
  - a double/triple bond only counts as one charge centre!
- Lone pairs / non-bonding pairs

## **VSEPR** Theory

- Example: ethyne
  - ► The carbon has two electron domains (the C-H bond and the C≡C bond)
  - They push as far away from each other as possible making a 180° bond angle





## Electron Domain Geometry vs Molecular Geometry

- Electron domain geometry: based on the total number of electron domains predicted from VSEPR Theory
- Molecular Geometry: gives the shape of the molecule

## **Basic Shapes**

Total Electron Domains	Electron- Domain Geometry	Bonding Domains	Non- bonding Domains	Molecular Geometry	Example	Main Angles
2 pairs	Linear	2	0	B-B Linear	ö=c=ö	180°
3 pairs	Trigonal planar	3	0	B B Trigonal planar	÷F: →B →F: →B →F: →F:	120 °
		2	1	Bent		118°
4 pairs	Tetrahedral	4	0	Tetrahedral	H H H H	109°
		3	1	Trigonal pyramidal	H H H	107 °
		2	2	Bent	н <mark>Ю</mark> .	105°

## Bond Angles in Molecular Geometries

- Lone pairs of electrons affect the bond angles in a molecule
- Lone pairs occupy more space than bonding pairs so they decrease the bond angle between bonding pairs
- LP|LP > LP|BP > BP|BP

## Problems to Try

1. SO<sub>2</sub>

- 2. CCl<sub>4</sub>
- 3. CHCl<sub>3</sub>
- 4. BF<sub>3</sub>
- 5. HCl



### **Resonance Structures**

Resonance structures occur when there is more than one possible position for a double bond in a molecule



## Problems to Try

## 1. NO<sub>3</sub><sup>-</sup>

## 2. CO<sub>3</sub><sup>2-</sup>

### 3. O<sub>3</sub>

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## Molecular Polarity

Bond polarity gives the polarity of individual bonds

- Molecular polarity tells whether the molecule itself is polar or nonpolar
- The polarity of molecules is distinct from the polarity of individual bonds
- A non-polar molecule may have polar bonds

## Molecular Polarity



## Problems to Try

1. SO<sub>2</sub>

- 2. CCl<sub>4</sub>
- 3. CHCl<sub>3</sub>
- 4. BF<sub>3</sub>
- 5. HCl



### Lesson 4

4.3 Covalent Structures





## Allotropes

 Allotropes are different structural modifications of the same elements

Allotropes can vary in physical and chemical properties

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### Carbon has a number of allotropes:

- Graphite
- Diamond
- Graphene
- C<sub>60</sub> fullerene

## **Covalent Network Solids**

- Carbon and silicon form giant covalent/network covalent structures
- Graphite, diamond, and graphene are examples of covalent network solids
- Quartz is a covalent network solid formed from silicon dioxide
- Covalent network solids are one in which the atoms are held together by covalent bonds in a giant three-dimensional lattice structure

## Properties of Covalent Network Solids

- Have high melting points (typically greater than 1000° C and much higher than the melting points of molecular structures)
- Poor electrical conductors (graphite and graphene are exceptions)
- Typically insoluble in common solvents

Hard solids

## Graphite

- Graphite contains layers of hexagonal rings consisting of carbon atoms
- These layers are connected by weak intermolecular forces of attraction, which are called London forces
- Graphite is used as a lubricant and in pencils (lead)
- Each carbon atom adopts a trigonal planar geometry, and is covalently bonded to three other carbon atoms at a bond angle of 120°.
- ► The layers are weak which allows the layers to slide past each other.

## Graphite



## Diamond

- Each carbon atom is covalently bonded to four other carbon atoms in a tetrahedral arrangement with a C-C-C bond angle of 109.5°.
- Diamond is one of the hardest substances because of the covalently bonded interlocking structural arrangement.
- Diamond is often used in heavy-duty cutting tools
- The strong covalent bonds do not allow the electrons to move freely, diamond does not conduct electricity
- Diamond is insoluble in all common solvents

## Diamond



### Graphene

- One of the thinnest and strongest of known materials
- ► The first two-dimensional crystal ever discovered
- Consists of a single planar sheet of carbon atoms arranged hexagonally, only one atom in thickness
- Each carbon atom is covalently bonded to three carbon atoms
- > The carbon atoms are densely packed in a honeycomb crystalline lattice

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- The experimental evidence for graphene was obtained in 2004
- It can be rolled up to form a nanotube

## Graphene

- Graphene is an excellent thermal and electrical conductor, 300 times more efficient than copper
- When graphite is picked apart it is essentially graphene
- When graphene is folded up into a sphere it becomes fullerene
- "New silicon"
- Future applications of graphene:
  - Development of graphene-plastic material to replace metals used in the aerospace industry because of their low density and high strength
  - Liquid crystal displays (LCD) and flexible touch screens for mobile devices due to flexibility, transparency, and electrical conductivity

## Graphene

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Discovered in 1985 at Rice University

- Fullerenes were found to form when vaporized carbon condensed in an atmosphere of inert gas
- The structure takes the shape of a soccer ball
- There are 20 hexagonal surfaces and 12 pentagonal surfaces
- Each carbon atom is covalently bonded to three others
- C<sub>60</sub> has been named buckminsterfullerene after the dome designed by a U.S. architect or referred to as buckyballs

C<sub>60</sub> fullerene is not a covalent network solid

- C<sub>60</sub> fullerene is composed of individual molecules with strong covalent bonds, but with weak London forces between the molecules
- Black solids that do not dissolve in water but can dissolve in some nonpolar solvents
- Can form colors ranging from red to brown to magenta
- Does conduct electricity

- Compounds of fullerenes have been synthesized as inclusion complexes, which can potentially be used as gene and drug carriers
- Other applications lie in the superconductivity and magnetic properties
- Fullerenes have the ability to fit inside the hydrophobic cavity that forms the active site of the human immunodeficiency virus (HIV) protease enzymes and inhibit them



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# SiO<sub>2</sub> (Quartz)

- Often called silica
- Amorphous in form-solid with no ordered structureas sand
- Consists of arrays of SiO<sub>2</sub> tetrahedra arranged in a lattice
- Each silicon atom is bonded covalently to four oxygen atoms and each oxygen atom is bonded covalently to two silicon atoms
- Bent Si-O-Si geometry
- High melting and high boiling point due to the strong covalent bonds

# SiO<sub>2</sub> (Quartz)

- Both crystalline and amorphous dioxide are insoluble in water
- Solid crystalline SiO<sub>2</sub> does not conduct electricity or heat
- Molten silicon dioxide can conduct electricity due to the movement of electrons
# $SiO_2$ (Quartz)



### **Coordinate Covalent Bonding**

- In coordinate covalent bonding, the shared pair of electrons comes from only one of the two atoms; this atom donates both electrons to the shared pair
- Arrows signify the origin of the electrons in the bond. Once formed all the bonds are equivalent.
- Examples:



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### **Coordinate Covalent Bonding**









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#### Lesson 4

4.4 Intermolecular Forces





### Intermolecular Forces

- The attractive forces between molecules
- It is these that are partially broken during melting, and fully broken during boiling
- Note: when molecular compounds melt/boil, the bonds in the molecule do not break, it is just the attractive forces *between* the molecules that break



### Types of Forces

#### Three main types:

- London Forces: also known as dispersion forces or instantaneous induced dipole-induced dipole forces
- Dipole-dipole forces
- Hydrogen bonding
- London forces + dipole-dipole forces + dipole-induced-dipole\* = van der Waals forces

#### Relative Strengths:

London forces < dipole-dipole forces < hydrogen bonds</p>

\*Dipole induced dipole is a weak attraction that results when a polar molecule induces a dipole in an atom or nonpolar molecule by disturbing the arrangement of electrons

#### <u>Main</u>

### London (Dispersion) Forces

- Random electron movements create a small, temporary dipole
- This induces a similar dipole in a neighbouring molecule
- This creates a small attraction between them
- These are weak and exist only for the tiniest fraction of a second
- London forces are present in all molecules
- London forces:
  - Increase with molecular mass



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### London (Dispersion) Forces

- Factors that affect the magnitude of London forces:
  - The number of electrons
    - The greater the number of electrons, the larger the distance between the valence electrons and the nucleus
    - The attraction of the valence electrons to the nucleus will be reduced and the electron cloud can be polarized more easily
  - The size (volume) of the electron cloud
    - In a large electron cloud, the attraction of electrons to the nucleus will not be as great as in a small electron cloud
    - The electrons in a large electron cloud can be polarized more easily
  - The shapes of the molecules
    - A higher contact area is much larger between molecules in a straight chain, London forces will have a greater magnitude

### Dipole-Dipole Forces

- Different atoms have different electronegativities, which means there will be variations in the electron charge density in different parts of a molecule
- If a molecule is not symmetrical, the variation produces a dipole where a molecule has a positive and a negative end
  - > The end with high charge density is  $\delta$ -
  - > The end with low charge density is  $\delta$ +
- Oppositely charged dipoles attract each other.

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This is a relatively strong attractive force







# Hydrogen Bonding

- The strongest type of intermolecular force
- They occur between a hydrogen that is bonded to a nitrogen, oxygen or fluorine
- N, O and F are the three most electronegative elements, and all have lone-pairs when bonded
- When H is bonded to N, O or F, the electrons bonded are strongly attracted to the N/O/F, leaving the H very positive

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The lone pair on the N/O/F is strongly attracted to the positive hydrogen





### Intermolecular Forces

	LONDON DISPERSION FORCES	DIPOLE-DIPOLE FORCES	HYDROGEN BONDING
Definition	<ul> <li>Attraction between 2 instantaneous dipoles.</li> <li>Asymmetrical electron distribution.</li> <li>All atoms &amp; molecules.</li> </ul>	<ul> <li>Attraction between 2 permanent dipoles.</li> <li>Polar molecules.</li> </ul>	<ul> <li>Attraction between molecules with N-H, O-H, &amp; F-H bonds.</li> <li>Extremely polar bonds ⇒ very strong dipole- dipole force.</li> </ul>
Diagram	$\delta^{-}$ $\delta^{+}$ $\delta^{-}$ $\delta^{+}$ H - H H - H	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	$\begin{array}{cccccccccccccccccccccccccccccccccccc$
Relative Strength	<ul> <li>weakest</li> </ul>	medium strength	<ul> <li>strongest</li> </ul>
Other Information	Increase in strength as molar mass increases (more electrons).	<ul> <li>Stronger when molecules are closer together</li> </ul>	Not chemical bonding.

Effects of intermolecular forces

- Intermolecular forces play an important role in the properties of compounds including:
  - Melting/boiling point:
    - Stronger intermolecular forces  $\rightarrow$  higher m.p./b.p.
  - Volatility:
    - Stronger intermolecular forces  $\rightarrow$  lower volatility
  - Solubility: like dissolves in like
    - Polar solutes dissolve best in polar solvents
    - Non-polar solutes dissolve best in non-polar solvents



van der Waals forces

### Determining Dipole

- 1. Identify polar bonds by comparing the electronegativities of the bonded atoms
- 2. Find the lone pairs of electrons
- 3. Determine if symmetry in the molecule balances out the positive and negative parts of the molecule
  - If the molecule is not symmetric in every direction, then it is polar.
  - Non-symmetric molecules have lone pairs on the central atom
  - The negative pole will be on the end of the molecule with the lone pairs or the end of the molecule with the most electronegative atom







### Examples







#### London forces only

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H is not bonded to O, N, or F so no hydrogen bonding

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#### London forces and dipole dipole



- Polar molecule
- H is not bonded to O, N, or F so no hydrogen bonding

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#### London forces and dipole dipole



► H is not bonded to O, N, or F so no hydrogen bonding

#### London forces and dipole dipole

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- H is bonded to so hydrogen bonding
- London forces, dipole dipole, hydrogen bonding

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#### Lesson 5

4.5 Metallic Bonding





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### Metallic Bonding

- A metallic bond is the electrostatic attraction between a lattice of positive ions and delocalized electrons
- The structure of a metal is a regular giant lattice that consists of positive ions surrounded by a "sea" of delocalized electrons



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### Metallic Bonding

- Delocalized electrons are not associated with a particular nucleus of a metal, but instead are free to move throughout the entire crystalline lattice forming a "sea" of mobile electrons
- The strength of a metallic bond depends on:
  - The number of valence electrons that can become delocalized
  - The charge of the metal ion
  - The ionic radius of the metallic positive ion

### Properties of Metallic Bonding

- Metals are good conductors of electricity because of the mobile delocalized electrons
- Metals are malleable: ability of a solid to be pounded or hammered into a sheet or other shape without breaking
- Malleability is due the positive ions the can slide past one another, which leads to a rearrangement of the shape of the solid

### Properties of Metallic Bonding

- Metallic bonds within the lattice do not have any defined direction: non-directional-act in every direction about the fixed immobile cations
- Very strong bond in metallic bonds leads to high melting points
- Melting point of metal depends on the strength of the attractive forces that hold the positive ions within the "sea" of delocalized electrons

### Melting Points of Metallic Bonds

- Melting point will decrease down a group with the decreasing strength of of the attractive forces
- Melting point will increase across a period from left to right
- Melting point trend is true for s and p blocks

### Melting Points of Metallic Bonds

- Calcium has 2 delocalized electrons per atom, whereas potassium has only one delocalized electron per atom
- The electrostatic attraction between the positive ions and the delocalized electrons will be greater in calcium

Element	Melting Point (K)	
Li	453	
Na	370	
К	336	
Rb	312	
Cs	301	
Fr	295	



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# Alloys

- An alloy is a mixture that contains either of two or more metals, or of a metal (or metals) combined with an alloying element composed of one or more nonmetals (ex: cast iron consists of the metal iron and the nonmetal carbon)
- major element: a metal + alloying element: can be a metal or nonmetal

### **Properties of Alloys**





# Alloys

- Properties of alloys in terms of non-directional bonding:
  - Greater strength
  - Greater resistance to corrosion
  - Enhanced magnetic properties
  - Greater ductility: property that allows a metal to deform under tensile stress (stretch into a wire)

### Alloys

- Adding a small amount of an alloying element can dramatically change the properties
- The availability of metal resources, and the means to extract them, varies greatly in different countries, and is a factor in determining national wealth. As technologies develop, the demands for different metals change and careful strategies are needed to manage the supply of these finite resources

### Lesson 6

#### 14.1 Further Aspects of Covalent Bonding and Structure





### Formal Charge

- Sometimes a number of different Lewis structures can be drawn that obey the octet rule.
- Formal charge is an approach in deciding which Lewis structure is the most appropriate.


Formal charge is the charge assigned to an atom in a molecule

### **Formal Charge**

 $FC = \frac{\# \text{ Valence } e^-}{\text{ in Free Atom}} - \frac{\text{ Total } \#}{\text{ Nonbonding } e^-} - \frac{\text{ Total } \#}{\frac{\text{ Bonding } e^-}{2}}$ 

If there are a number of possible Lewis structures that all obey the octet rule, the most reasonable one will be

- The one the FC difference closest to O
- The one that has the negative charges located on the most electronegative atoms



► ΔFC = 0

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FC(B) = 
$$(3) - (0) - \frac{1}{2}(6) = 0$$

FC(F) = 
$$(7) - (6) - \frac{1}{2}(2) = C$$





FC(B) = 
$$(3) - (0) - \frac{1}{2}(8) = -1$$

FC(
$$F_A$$
) = (7) - (4) -  $\frac{1}{2}$ (4) = +1

► 
$$FC(F_B) = (7) - (6) - \frac{1}{2}(2) = 0$$

• 
$$\Delta FC = FC_{max} - FC_{min} = (+1) - (-1) = +2$$



**Formal Charge** 

Consider nitrosyl chloride, NOCI

	:CI≕N-Ö:	∶ĊI—N=O.	
CI	7 – (2+4) = +1	CI	7 – (1+6) = 0
Ν	5 - (3+2) = 0	Ν	5 - (3+2) = 0
0	6 - (1+6) = -1	0	6 - (2+4) = 0

### Molecular Geometries

Electron Domains	Electron-Domain Geometry	Bonding Domains	Nonbonding Domains	Molecular Geometry	Example
5 domains		5	0	B B B B	PCl <sub>5</sub>
	Trigonal bipyramidal			Trigonal bipyramidal	
		4	1	Soocaw	$SF_4$
		3	2	Secsaw B	CIF <sub>3</sub>
		2	3	T-shaped	XeF <sub>2</sub>
6 domains		6	o	B B B B	SF <sub>6</sub>
	Octahedral	5	1	Octahedral	BrF <sub>5</sub>
				Square pyramidal	
		4	2	B B B	XeF <sub>4</sub>
				planar	

# Sigma and Pi Bonds

- Covalent bonds result from the overlap of atomic orbitals. A sigma bond is formed by the direct head-on/end-to-end overlap of atomic orbitals, resulting in electron density concentrated between the nuclei of the bonding atoms.
- A pi bond is formed by the sideways overlap of atomic orbitals, resulting in electron density above and below the plane of the nuclei of the bonding atoms.



### Sigma and Pi Bonds

Linear combination of atomic orbitals.

Single Covalent Bond	1 sigma bond
Double Covalent Bond	1 sigma, 1 pi bond
Triple Covalent Bond	1 sigma, 2 pi bonds



### Sigma-bonds/ $\sigma$ -bonds

- σ-bonds are formed when two orbitals from neighbouring atoms overlap along the axis of approach
- Viewed end on, σ-bonding orbitals appear circular



Formation of a sigma bond due to (a) The s - s overlap (b) The s - p overlap (c) The p<sub>z</sub> - p<sub>z</sub> overlap

# Pi-bonds/ $\pi$ -bonds

 π-bonds are formed when two orbitals from neighbouring atoms overlap perpendicular to the axis of approach



- Viewed end on, π-bonds orbitals appear as two circles, one above the atoms and one below
- π -bonds make up the second and third bonds of double and triple bonds
- $\pi$  -bonds are weaker than  $\sigma$ -bonds due to the weaker overlap of the orbitals

### Delocalization

 Delocalization involves electrons that are shared by/between more than one pair in a molecule or ion as opposed to being localized between a pair of atoms.



### Delocalization

- A resonance structure is one of two or more alternative Lewis (electron dot) structures for a molecule or ion that cannot be described fully with one Lewis (electron dot) structure alone.
- Delocalization makes species more stable by spreading out the electron charge making it less attractive to positive attackers (electrophiles)
  - It is the stability of benzene that makes it such a serious carcinogen

### Bond Order





### Ozone and Oxygen

- Ozone and oxygen play an important role in protecting the surface of the Earth from damaging effects of ultraviolet radiation
- UV radiation is absorbed by molecules or O<sub>2</sub> or O<sub>3</sub> as they dissociate
- The highest energy UV radiation is absorbed by O<sub>2</sub>



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### Wavelength of Light to Dissociate Oxygen and Ozone

The bonds in ozone can be broken by UV radiation

- The bond order in ozone is lower than the bond order in oxygen, so the double bond in oxygen is stronger
- Radiation of shorter wavelength is required to break the stronger bond in oxygen
- The energy is inversely proportional to the wavelength, the greater the energy the shorter the wavelength



### **Ozone Depletion**



The average bond enthalpy in ozone is 362 kJ mol<sup>-1</sup>. Using the relationships given in section 1 and the bond enthalpy in section 11 of the Data Booklet, calculate the maximum wavelength, in nm, of the UV radiation required to break the O=O double bond and the O-O bond in ozone.

- Oxygen:
  - The bond enthalpy for O=O is 498 kJ mol<sup>-1</sup>.
- Convert kJ to J
  - 498 x 1000 kJ mol<sup>-1</sup>

6.02 x 10<sup>23</sup> mol<sup>-1</sup>

- Solve for wavelength using E = hv
  - λ = hc/E
  - ► (6.63 x 10-<sup>34</sup>J s) x (3.00 x 10<sup>8</sup>m/s) / (8.27 x 10<sup>-19</sup>J)
- Convert m to nm
  - (2.41 x 10<sup>-7</sup>m) x (1nm/ 10<sup>-9</sup>m)
- Wavelength = 241nm

- Ozone:
  - ▶ The bond enthalpy for O-O is 362 kJ mol<sup>-1</sup>.
- Convert kJ to J
  - ▶ 362 x 1000 kJ mol<sup>-1</sup>
    - 6.02 x 10<sup>23</sup> mol<sup>-1</sup>
- Solve for wavelength using E = hv
  - λ = hc/E
  - $(6.63 \times 10^{-34} \text{J s}) \times (3.00 \times 10^8 \text{m/s}) / (6.01 \times 10^{-19} \text{J})$
- Convert m to nm
  - ▶ (3.31 x 10<sup>-7</sup>m) x (1nm/ 10<sup>-9</sup>m)
- Wavelength = 331nm

### Lesson 7

14.2 Hybridization





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### Hybridization

- A hybrid orbital results from the mixing of different types of atomic orbitals on the same atom.
- Hybridization in which s and p orbitals merge together to create new atomic orbitals
- We need to know about three types of hybridization:
  - $\triangleright$  sp<sup>3</sup>
  - ► sp<sup>2</sup>
  - sp sp

sp<sup>3</sup> hybridization

- One 's' orbital combines with three 'p' orbitals to create four 'sp<sup>3</sup>' orbitals
- The sp<sup>3</sup> orbitals are arranged tetrahedrally
- Most atoms with tetrahedral geometry will be sp<sup>3</sup> hybridized



sp<sup>2</sup> hybridization

- One 's' orbital combines with two 'p' orbitals to create three 'sp<sup>2</sup>' orbitals, leaving one 'p' orbital untouched
- The sp<sup>2</sup> orbitals have a trigonal planar arrangement
- Most atoms with trigonal planar geometry will be sp<sup>2</sup> hybridized



### sp hybridization

- One 's' orbital combines with one 'p' orbital to create two 'sp' orbitals and leaving two 'p' orbitals untouched
- The sp orbitals have a linear arrangement
- Most atoms with linear geometry will be sp hybridized



Hybridization						
	coordination # + # lone pairs = n					
	Table 4					
n	hybridization	electron-pair geometry				
4	sp <sup>3</sup>	tetrahedral				
3	sp <sup>2</sup>	planar trigonal				
2	sp	linear				