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## Chapter 2

# Atoms and Molecules

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## Warning!!

- These slides contains visual aids for learning BUT they are NOT the actual lecture notes!
- Failure to attend to lectures most probably result in failing the lecture!
- So I strongly recommend that you attend to the classes. Take a pen, a notebook and WRITE!

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## Chapter Objectives

- Name at least three common polymers and give examples of their uses.
- Define the terms *atom*, *molecule*, *isotope*, *ion*, *polymer*, *monomer*, and *functional group* in your own words.
- Describe the *nuclear model* for the atom and identify the numbers of *protons*, *electrons*, and *neutrons* in a particular isotope from its chemical symbol.
- Calculate the *atomic mass* of an element from the masses and abundances of its isotopes.

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## Chapter Objectives

- Explain the difference between a *molecular formula* and an *empirical formula*.
- Determine the number of atoms in a molecule from its chemical formula.
- Describe the arrangement of elements in the *periodic table* and explain the usefulness of the table.
- Determine the correct chemical formula from a *line drawing* of an organic molecule.

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## Chapter Objectives

- Use standard *chemical nomenclature* to deduce the names of simple inorganic compounds from their formulas or *vice versa*.
- Describe different forms of polyethylene and how their properties and applications are related to their molecular structure.


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## Polymers

- *Polymers* are very large molecules made up of many smaller molecules linked together.
- *Monomers* - The small molecules linked together in polymers.
- *Polymer backbone* - The long chain of bonded atoms formed when monomers link together to form polymers.

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## Polymers

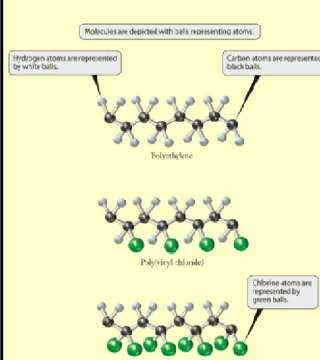


(a) (b) (c)

- Polymers are the materials of choice for a host of everyday objects.
  - polyethylene
  - polystyrene
  - poly(vinyl chloride), PVC

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## Polymers



Molecules are depicted with balls representing atoms.

Hydrogen atoms are represented by white balls.

Carbon atoms are represented by black balls.

Chlorine atoms are represented by green balls.

- Models showing how atoms are arranged in several polymers.
- Each of these polymers has distinct properties.

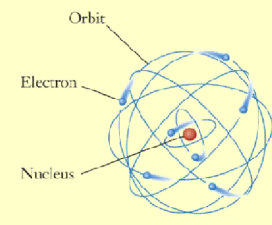
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## Atomic Structure and Mass

- Matter is composed of atoms.
  - Atoms have a **nucleus** which contains **protons** and **neutrons**.
  - The nucleus is surrounded by a cloud of **electrons**.
  - The nucleus is a very small fraction of the volume of an atom.

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## Fundamental Concepts of the Atom

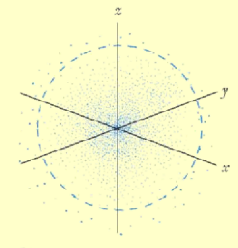


(a)

- Solar system depiction of atomic structure.
  - Emphasizes proton, neutron and electron distribution; *does not accurately depict current accepted model of atomic structure.*

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## Fundamental Concepts of the Atom



(b)

- Electrons are depicted as **clouds** of negative charge surrounding the nucleus.
  - The density of the small dots is related to the probability of finding an electron at a particular location.

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## Atomic Number and Mass Number

- Atomic Number,  $Z$** , is the number of protons in a nucleus.
  - identifies the element
- Mass Number,  $A$** , is the sum of the number of protons and number of neutrons in a nucleus.

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## Atomic Number and Mass Number

- 1 amu =  $1.6605 \times 10^{-24}$  g
- Protons and neutrons are nearly 2000 times more massive than electrons

Particle	mass (amu)	charge
Proton	1.007	+
Neutron	1.009	0
Electron	0.00055	-

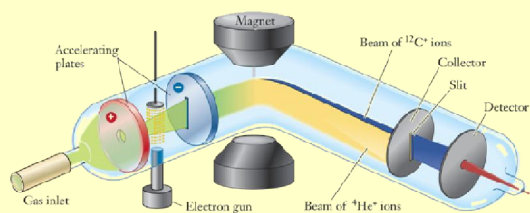
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## Isotopes

- **Isotopes** are atoms of an element that differ in the number of neutrons in their nucleus.
  - same Z but different A
- **Isotopic abundance** is the mass percentage of an isotope in a naturally occurring element.

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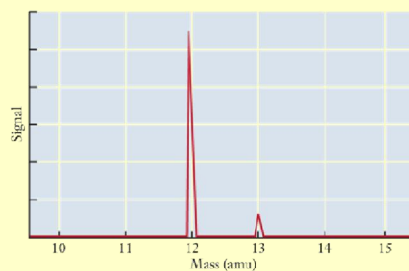
## Isotopes



- Mass spectrometers can measure the masses of atoms, isotopes, and molecules.

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## Isotopes



- Mass spectrum showing carbon isotopes.

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## Atomic Symbols

- Information regarding atomic structure is written in scientific shorthand called the atomic symbol.



- E is the atomic symbol for element
- Superscript A is the mass number.
- Subscript Z is the atomic number.

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## Atomic Symbols

Table 2.1

Names and symbols of some common elements whose symbols are not related to their English names

Name	Symbol (name origin)
Gold	Au (aurum)
Iron	Fe (ferrum)
Lead	Pb (plumbum)
Mercury	Hg (hydrargyrum)
Silver	Ag (argentum)
Sodium	Na (natrium)

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## Atomic Masses

6  
C  
12.011

Atomic number

Symbol

Relative atomic mass

- Entry for carbon on the periodic table.
- $Z = 6$
- Relative atomic mass = 12.011 (~99% carbon-12)
- Element Symbol: C

$^{12}_6\text{C}$

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## Atomic Masses

- **Relative atomic mass** for an element is an *average* of the atomic masses for the naturally occurring isotopes for an element.
- Carbon-12 =  $12.0000 \times 0.9893 = 11.871$  amu
- Carbon-13 =  $13.0036 \times 0.0107 = 0.1391$  amu
- Average mass =  $11.87 + 0.139 = 12.01$  amu

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## Example Problem 2.1

- The chlorine present in PVC has two stable isotopes:  $^{35}\text{Cl}$ , with a mass of 34.97 amu and 75.77% abundance; and  $^{37}\text{Cl}$ , with a mass of 36.95 amu. What is the atomic mass of chlorine?

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## Ions

- Ions are formed when the number of protons and electrons in an atom are not equal.
  - Ions with more protons than electrons are called **cations**.
    - net positive charge
  - Ions with more electrons than protons are called **anions**.
    - net negative charge
- A **monatomic ion** is derived from a single atom.
- A **polyatomic ion** is derived from a group of atoms with an overall charge.

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## Ions

**Table 2.2**

Examples of monatomic ions

Cation Name	Symbol	Anion Name	Symbol
Sodium ion	$\text{Na}^+$	Fluoride ion	$\text{F}^-$
Lithium ion	$\text{Li}^+$	Chloride ion	$\text{Cl}^-$
Potassium ion	$\text{K}^+$	Bromide ion	$\text{Br}^-$
Magnesium ion	$\text{Mg}^{2+}$	Sulfide ion	$\text{S}^{2-}$
Aluminum ion	$\text{Al}^{3+}$	Nitride ion	$\text{N}^{3-}$

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## Mathematical Description

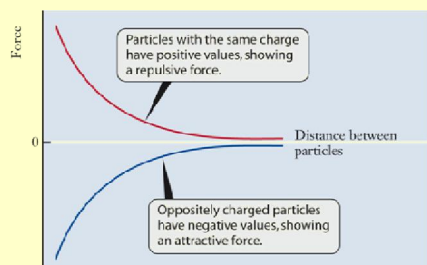
- **Coulombs' Law** states that the force between ions is proportional to the product of the ion charges divided by distance squared.

$$F = \frac{q_1 q_2}{4\pi\epsilon_0 r^2}$$

- Opposite charges attract and like charges repel.
  - $q_1$  and  $q_2$  are charges;  $\epsilon_0$  and  $\pi$  are constants;  $r$  is the distance between the charges
- Electric charge is conserved.

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## Mathematical Description



- The electrical force varies with the distance,  $r$ , between charged particles.

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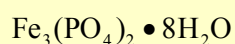
## Ions and Their Properties

- An element and its ion have the same chemical symbol but different properties.
  - Sodium metal atoms lose an electron to form sodium cations.
    - Sodium metal reacts violently with water.
  - Chlorine gas molecules gain electrons to form chlorine anions (chloride).
    - Chlorine gas reacts violently with sodium metal.
- Ionic compounds containing sodium cation and chlorine anion dissolve in water without reacting.

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## Chemical Formulas

- Chemical formulas** describe a compound in terms of the elements the compound contains.
  - The number of atoms for each element is indicated by a subscript to the right of the chemical symbol.
    - Groups of atoms can be designated using parentheses. Subscripts outside these parentheses mean that all atoms enclosed in the parentheses are multiplied by the value indicated by the subscript.
  - Water molecules associated with certain compounds, called **hydrates**, are indicated separately from the rest of the compound.



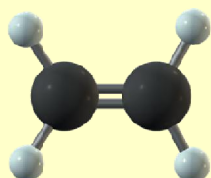
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## Chemical Formulas

- Compounds** have different properties than their constituent atoms.
- Ionic compounds** contain cations and anions, usually arranged in a lattice.
- Molecular formulas** indicate the elements and number of atoms of each element actually contained in a discrete unit of a compound.
- Empirical formulas** indicate the smallest whole number ratio between the number of atoms of each element in a molecular formula.

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## Chemical Formulas

Ethylene,  $\text{C}_2\text{H}_4$ 

- The molecular formula for ethylene is  $\text{C}_2\text{H}_4$ .
- The empirical formula for ethylene is  $\text{CH}_2$ .
- Polyethylene can be written as  $-\text{[CH}_2\text{CH}_2\text{]}_n-$ 
  - $n$  is used to emphasize that a large number of these units are found in an individual molecule

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## Example Problem 2.2

- One polymerization initiator is diethylaluminum chloride,  $\text{Al}(\text{C}_2\text{H}_5)_2\text{Cl}$ . How many of each type of atom are in a molecule of this compound?

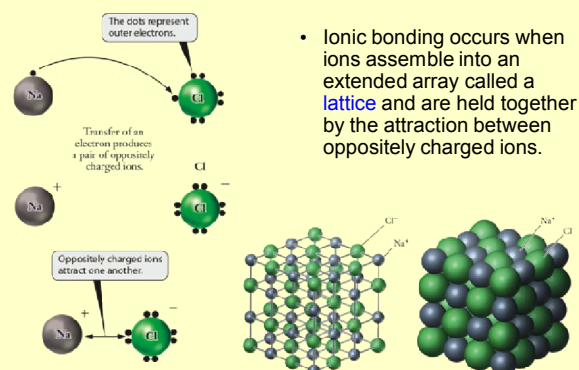
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## Chemical Bonding

- All bonds are created by the **exchange** or **sharing** of electrons.
- The exchange or sharing of electrons results in lower energy for the compound relative to the separate atoms.
  - Ionic:** exchange; cations and anions present
  - Metallic:** sharing by forming a mobile "sea of electrons"
  - Covalent:** sharing between atoms

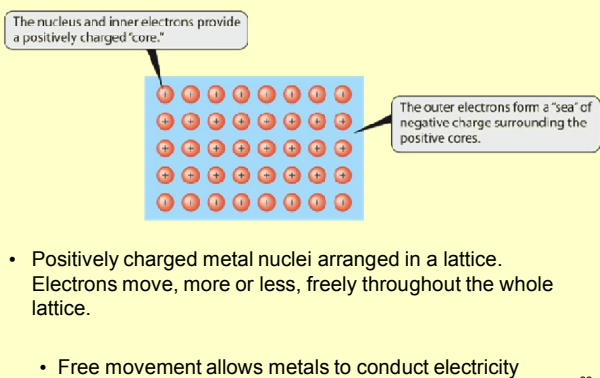
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## Ionic Bonding



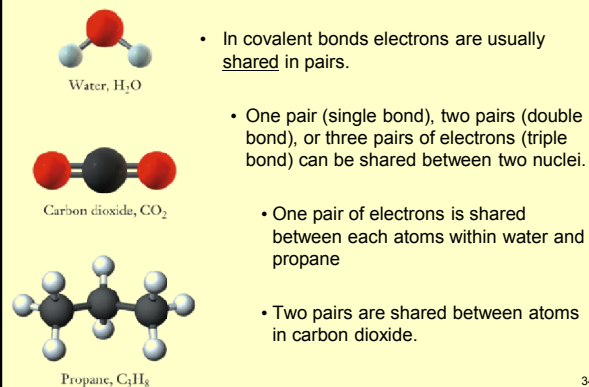
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## Metallic Bonding



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## Covalent Bonding



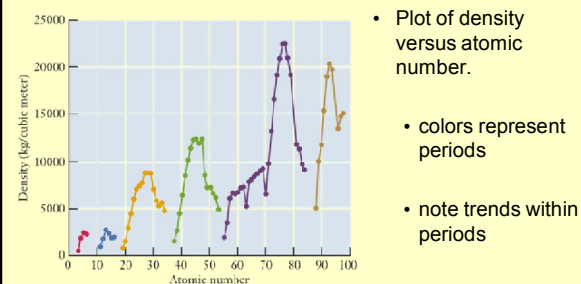
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## The Periodic Table

- The **Periodic Table** is based on periodic law.
- Periodic law** - when arranged properly, the elements display a regular and periodic variation in their chemical properties.
  - Periods** are **horizontal** rows on the periodic table.
  - Groups** are **vertical** columns on the periodic table.

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## Periods and Groups



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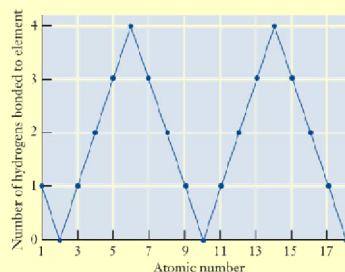
## Periods and Groups

1																	17	18
H	2											B	C	N	O	F	Ne	
Li	Be											Al	Si	P	S	Cl	Ar	
Na	Mg	3	4	5	6	7	8	9	10	11	12	Ga	Ge	As	Se	Br	Kr	
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	In	Sn	Sb	Te	I	Xe	
Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	Hg	Tl	Pb	Bi	Po	At	Rn
Cs	Ba	La	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn	
Fr	Ra	Ac	Rf	Hf	Sg	Ns	Hs	Mt										
		Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu			
		Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr			

- Density data presented with shading.

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## Periods and Groups



- Graph of the number of hydrogen atoms with which an individual atom of various elements will combine.

- another periodic trend

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## Periods and Groups

- Common names of specific groups:
  - Group 1: **alkali metals**.
  - Group 2: **alkaline earth metals**.
  - Group 17: **halogens**.
  - Group 18: **noble gases/rare gases**.
- Table Regions:
  - Groups 1-2 and 13-18 are **main group elements**
  - Groups 3-12 are **transition metals**
  - Lanthanides** and **actinides** are below the rest of the table

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## Metals, Nonmetals, and Metalloids

- Metals** are generally toward the left and bottom of the periodic table. They are shiny, malleable, and ductile. They conduct current and easily form cations.
- Nonmetals** occupy the upper right-hand portion of the periodic table. They are not shiny, malleable, or ductile. They do not conduct current but do easily form anions.
- Metalloids**, or **semimetals**, have chemical properties intermediate of metals and nonmetals. Metalloids are clustered along a diagonal line on the periodic table between the metals and nonmetals.

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## Metals, Nonmetals, and Metalloids

1																	17	18
H	2											B	C	N	O	F	Ne	
Li	Be											Al	Si	P	S	Cl	Ar	
Na	Mg	3	4	5	6	7	8	9	10	11	12	Ga	Ge	As	Se	Br	Kr	
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	In	Sn	Sb	Te	I	Xe	
Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	Hg	Tl	Pb	Bi	Po	At	Rn
Cs	Ba	La	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn	
Fr	Ra	Ac	Rf	Hf	Sg	Ns	Hs	Mt										
		Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu			
		Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr			

Metals  
 Metalloids  
 Nonmetals

blue = metals, orange = metalloids, purple = nonmetals

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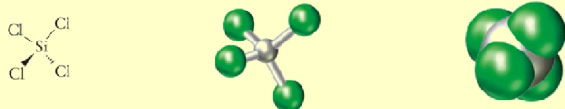
## Inorganic and Organic Chemistry

- Organic chemistry** is the study of the compounds of the element carbon, usually with oxygen, nitrogen, and hydrogen.
  - More than 18 million organic compounds exist.
  - Includes biological molecules and nearly all synthetic polymers.
  - Isomers**: Different organic molecules that have the same formula but are connected differently.
- Inorganic chemistry** is the study of all other elements and their compounds.

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## Inorganic Chemistry - Main Group and Transition Metals

- Many main group inorganic compounds exist as relatively small molecules whose atoms are joined together through covalent bonds.



- Other main group compounds form extended ionic structures, such as that of NaCl.

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## Inorganic Chemistry - Main Group and Transition Metals



Iron(III) chloride,  $FeCl_3$   
(Here forming as the solid at the bottom of the test tube)  
Orange-brown color  
Density  $2.90 \text{ g cm}^{-3}$   
Melts at  $306^\circ\text{C}$



Iron(II) chloride,  $FeCl_2$   
Greenish-yellow color  
Density  $3.16 \text{ g cm}^{-3}$   
Melts at  $670^\circ\text{C}$

- Transition metal cations have variable charge, resulting in a variety of compounds with different chemical and physical properties.
- Transition metal chemistry is more complicated than main group metal chemistry.

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## Organic Chemistry

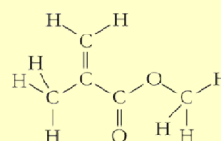
- Because carbon compounds can become quite large, organic compounds are described simply and unambiguously using **line structures**, where carbons and hydrogens are not explicitly shown.
  - Each corner or end of a line is a carbon.
  - Hydrogen atoms on carbon atoms are implied. Carbon makes four bonds, "missing" bonds go to hydrogen atoms. Hydrogen can only make one covalent bond to another atom.
  - Hydrogen atoms on any other element are shown
  - All other elements are shown



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## Example Problem 2.3

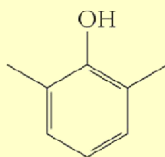
- The structural formula for methyl methacrylate, the monomer unit of Plexiglas<sup>®</sup>, is shown below. Write the corresponding line structure for this compound.



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## Example Problem 2.4

- The line structure below represents 2,6-dimethylphenol. What is its molecular formula?



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## Functional Groups

- Functional groups** are arrangements of atoms that tend to display similar chemical properties.
  - Chemical formulas are often written to emphasize functional groups.
    - Methanol, an alcohol, is often written  $CH_3OH$  instead of  $CH_4O$ .
- Hydrocarbons** contain only H and C atoms.
  - Addition of functional groups to hydrocarbons results in more complex compounds.




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## Functional Groups

Table 2.3

Some common functional groups





Functional Group	Class of Compounds	Example
	Alkenes	Ethylene
	Alkynes	Acetylene
$-X$ (X = F, Cl, Br, I)	Organic halides	Methyl chloride
$-OH$	Alcohols, phenols	Ethanol, phenol
$C-O-C$	Ethers	Diethyl ether
	Amines	Methylamine

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## Functional Groups

Table 2.3 (continued)

Some common functional groups

Functional Group	Class of Compounds	Example
	Carboxylic acids	Acetic acid
	Amides	Acetanilide
	Aldehydes	Formaldehyde
	Ketones	Methyl ethyl ketone

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## Chemical Nomenclature

- **Chemical nomenclature** is a systematic means of assigning names to chemical compounds.
- **Binary compounds** contain only two elements.
  - Covalent binary compounds are named differently from ionic binary compounds.
  - Recognizing a compound as ionic or covalent assists in naming.
    - A metal and a nonmetal generally combine to form ionic compounds.
    - Two nonmetals generally combine to form a covalent compound.
    - Presence of polyatomic ions indicates ionic bonding.

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## Naming Covalent Compounds

- The first element in the formula retains its full name.
- The second element is named by replacing the ending from its name with the suffix *-ide*.
- Both elements are preceded by a number-designating prefix except when there is only one atom of the first element, which will not use the prefix *mono-*.

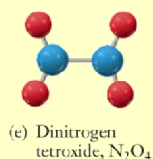
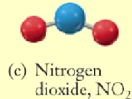
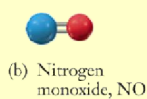
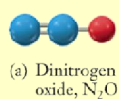
Table 2.4

Greek prefixes for the first ten numbers

Number	Prefix
One	Mono-
Two	Di-
Three	Tri-
Four	Tetra-
Five	Penta-
Six	Hexa-
Seven	Hepta-
Eight	Octa-
Nine	Nona-
Ten	Deca-

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## Naming Covalent Compounds



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## Example Problem 2.5

- What are the systematic names of the following compounds?
  - $N_2O_5$
  - $PCl_3$
  - $P_4O_6$

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## Naming Ionic Compounds

- Ionic compounds are electrically neutral and are named in order of "cation anion", as in sodium chloride.
  - The cation retains its full name.
    - Monoatomic cation charge can often be found by position in the periodic table.
    - Cations with more than one charge (e.g., transition metals) are named using Roman numerals indicating the charge, e.g., iron(II)
  - Monatomic anions are named by replacing the ending of the element name with the suffix *-ide*, e.g., *bromide*
  - A polyatomic cation or anion is named using its common name.

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## Naming Ionic Compounds

Table 2.5

## Common cations

Sodium ion	Na <sup>+</sup>	Potassium ion	K <sup>+</sup>
Magnesium ion	Mg <sup>2+</sup>	Calcium ion	Ca <sup>2+</sup>
Iron(II) ion	Fe <sup>2+</sup>	Copper(I) ion	Cu <sup>+</sup>
Iron(III) ion	Fe <sup>3+</sup>	Copper(II) ion	Cu <sup>2+</sup>
Silver ion	Ag <sup>+</sup>	Zinc ion	Zn <sup>2+</sup>
Ammonium ion	NH <sub>4</sub> <sup>+</sup>	Hydronium ion	H <sub>3</sub> O <sup>+</sup>

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## Naming Ionic Compounds

Table 2.6

## Common anions

Halides	F <sup>-</sup> , Cl <sup>-</sup> , Br <sup>-</sup> , I <sup>-</sup>	Sulfate	SO <sub>4</sub> <sup>2-</sup>
Nitrate	NO <sub>3</sub> <sup>-</sup>	Hydroxide	OH <sup>-</sup>
Phosphate	PO <sub>4</sub> <sup>3-</sup>	Cyanide	CN <sup>-</sup>
Carbonate	CO <sub>3</sub> <sup>2-</sup>	Hydrogen carbonate	HCO <sub>3</sub> <sup>-</sup>

- The charge and chemical formula for each polyatomic ion should be memorized.

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## Naming Ionic Compounds

Table 2.7

## Oxyanions of chlorine

ClO <sup>-</sup>	Hypochlorite
ClO <sub>2</sub> <sup>-</sup>	Chlorite
ClO <sub>3</sub> <sup>-</sup>	Chlorate
ClO <sub>4</sub> <sup>-</sup>	Perchlorate

- Polyatomic ions containing oxygen and another element are **oxyanions**.
  - Base name provided by element that is not oxygen.
    - For two possible groupings, the one with more oxygen atoms uses the suffix *-ate*, the one with fewer oxygen atoms uses the suffix *-ite*.
    - For four groupings, the prefix *per-* is added to *-ate* for the compound with the most oxygen atoms.
    - The prefix *hypo-* is added to *-ite* for the compound with the least oxygen atoms.

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## Example Problem 2.6

- Determine the names of the following ionic compounds:
  - Fe<sub>2</sub>O<sub>3</sub>
  - Na<sub>2</sub>O
  - Ca(NO<sub>3</sub>)<sub>2</sub>

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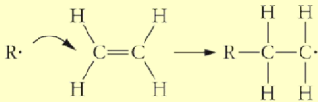
## Polyethylene

- Polyethylene is one of the most common polymers in the world.
  - US production in 2007 was more than 39 billion pounds.
- Polyethylene  $-\text{[CH}_2\text{CH}_2\text{]}_n-$  is built from the monomer ethylene, C<sub>2</sub>H<sub>4</sub>.

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## Polyethylene

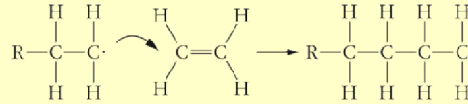
- Ethylene monomers are linked together via a free radical mechanism, which converts the carbon-carbon double bond to a single bond.
- Free radicals** have an unshared single electron and are extremely reactive.
- An **initiator** produces the free radical that reacts with ethylene, opening the double bond and transferring the free radical to the ethylene monomer.



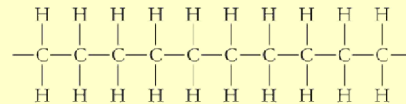
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## Polyethylene

- The ethylene free radical reacts with another ethylene monomer, extending the polyethylene chain.

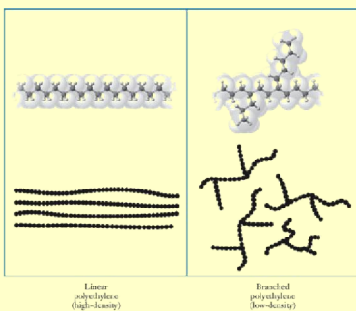


- Polymerization continues until the free radical reacts with another free radical, or terminator, which terminates the growth of the chain.



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## Polyethylene



- Polyethylene polymers can be linear chains (high-density polyethylene, HDPE) or branched chains (low-density polyethylene, LDPE).
- Ultra-high molecular weight polyethylene, UHMWPE, contains extremely long chains.

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