Chemical Bonds, Chemical Compounds, and Chemical Weapons

http://preparatorychemistry.com/Bishop_Book_atoms_5.pdf



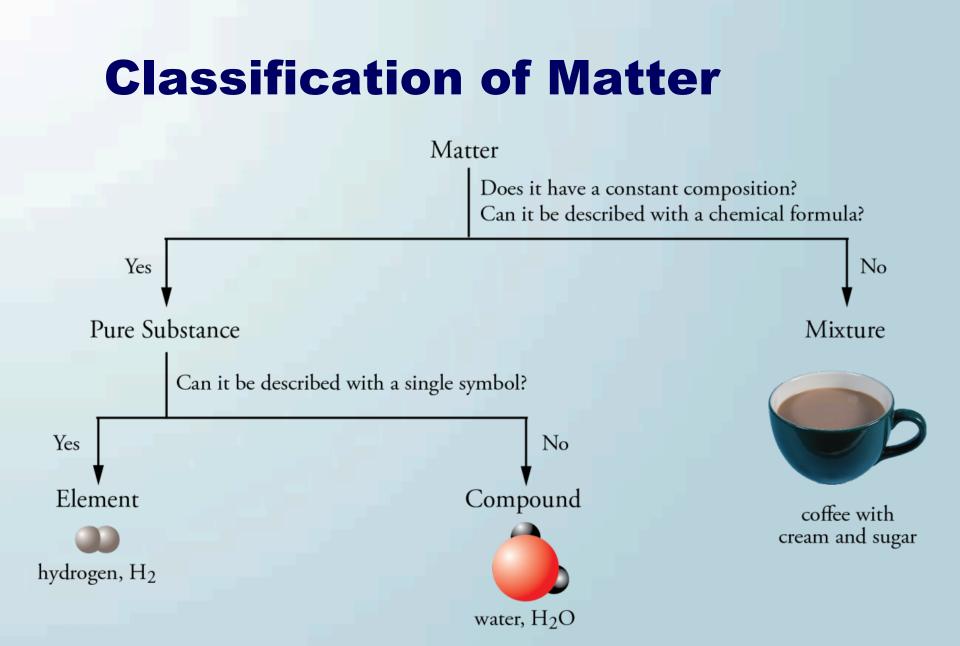
Elements, Compounds, and Mixtures

- Element: A substance that cannot be chemically converted into simpler substances; a substance in which all of the atoms have the same number of protons and therefore the same chemical characteristics.
- Compound: A substance that contains two or more elements, the atoms of these elements always combining in the same whole-number ratio.
- **Mixture:** A sample of matter that contains two or more pure substances (elements and compounds) and has variable composition.

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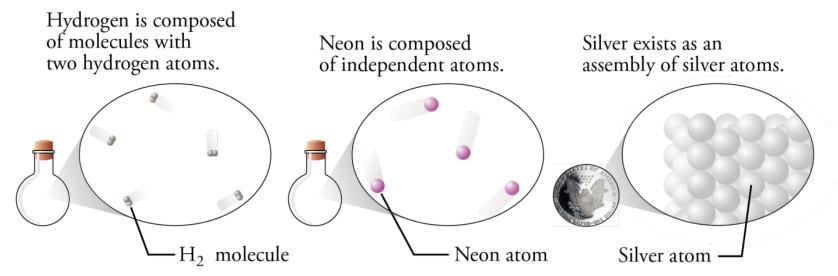
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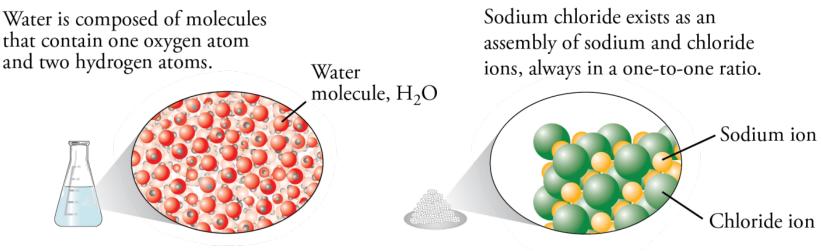


Elements and Compounds

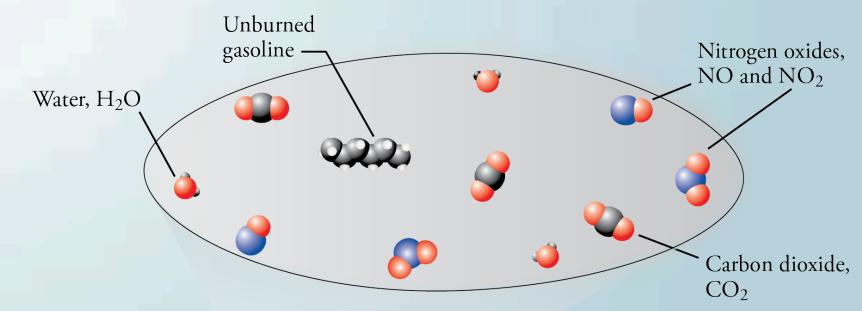
ELEMENTS



COMPOUNDS



Exhaust – a Mixture





Covalent Bond Formation

Hydrogen nuclei

Two hydrogen atoms interact to form one hydrogen molecule

Covalent Bond

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- A link between atoms due to the sharing of two electrons. This bond forms between atoms of two nonmetallic elements.
 - If the electrons are shared equally, there is a even distribution of the negative charge for the electrons in the bond, so there is no partial charges on the atoms. The bond is called a *nonpolar covalent bond*.
 - If one atom in the bond attracts electrons more than the other atom, the electron negative charge shifts to that atom giving it a partial negative charge. The other atom loses negative charge giving it a partial positive charge. The bond is called a *polar covalent bond*.

Polar Covalent Bond

δ+

H

Electrons shift toward the chlorine atom, forming partial plus and minus charges.

 \mathbf{Cl}

Hydrogen attracts electrons less.

Chlorine attracts electrons more.

δ-

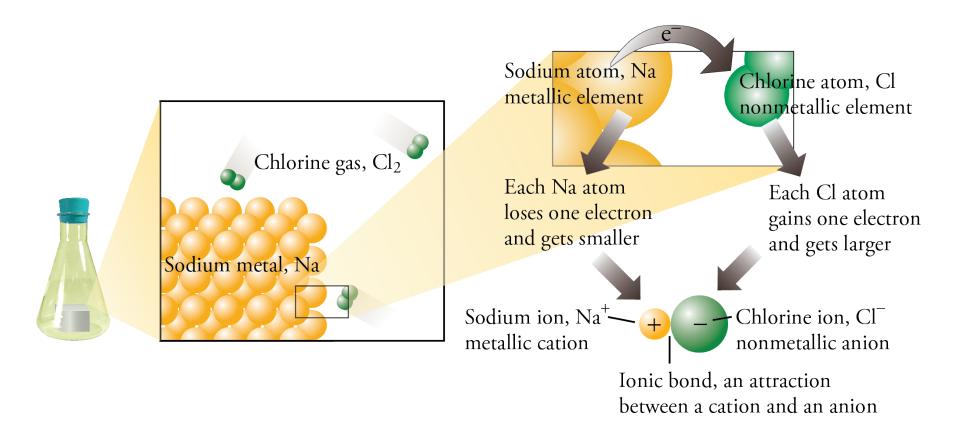
Ionic Bond

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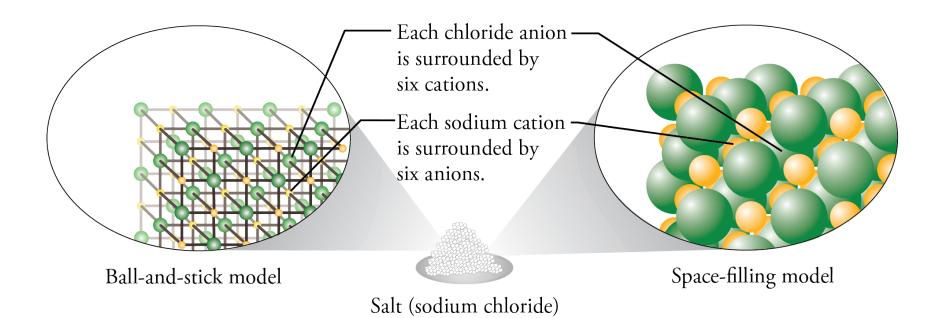
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- The attraction between cation and anion.
- Atoms of nonmetallic elements often attract electrons so much more strongly than atoms of metallic elements that one or more electrons are transferred from the metallic atom (forming a positively charged particle or *cation*), to the nonmetallic atom (forming a negatively charged particle or *anion*).
- For example, an uncharged chlorine atom can pull one electron from an uncharged sodium atom, yielding Cl⁻ and Na⁺.

Ionic Bond Formation



Sodium Chloride, NaCl, Structure

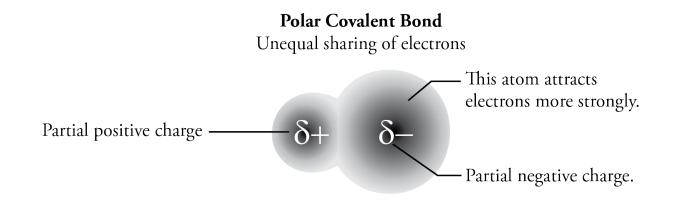


Bond Types

Nonpolar Covalent Bond

Equal sharing of electrons

Both atoms attract electrons equally (or nearly so). No significant charges form.



Ionic Bond

Strong attraction between positive and negative charges.

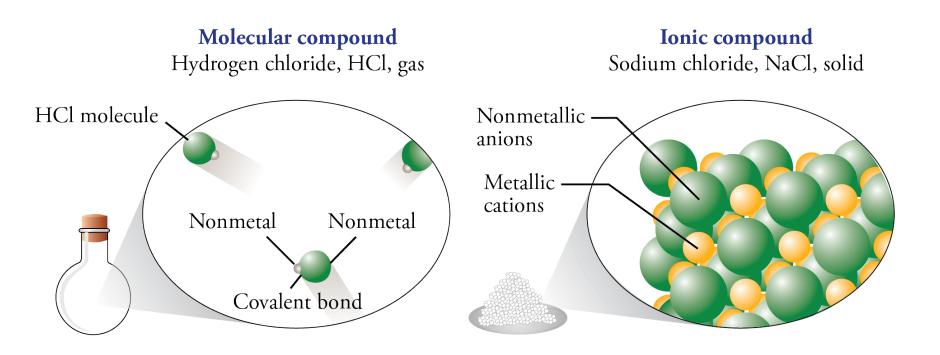
This atom loses one or more electrons and gains a positive charge. — + / — Ionic bond This atom attracts electrons so much more strongly than the other atom that it gains one or more electrons and gains a negative charge.

Types of Compounds

- All nonmetallic atoms usually leads to all covalent bonds, which from molecules. These compounds are called *molecular compounds*.
- Metal-nonmetal combinations usually lead to ionic bonds and *ionic compounds*.

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Classification of Compounds



Summary

- Nonmetal-nonmetal combinations (e.g. HCI)
 - Covalent bonds
 - Molecules

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- Molecular Compound
- Metal-nonmetal combinations (e.g. NaCl)
 - Probably ionic bonds
 - Alternating cations and anions in crystal structure
 - Ionic compound

Valence Electrons

- The valence electrons for each atom are the most important electrons in the formation of chemical bonds.
- The number of valence electrons for the atoms of each element is equal to the element's A-group number on the periodic table.
- Covalent bonds often form to pair unpaired electrons and give the atoms of the elements other than hydrogen and boron eight valence electrons (an octet of valence electrons).

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Valence Electrons and A-Group Numbers

One valence electron

Η

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Number of valence electrons equals the A-group number						
3A	4A	5A	6A	7A	2 He	
5 B	6 C	7 N	8 O	9 F	10 Ne	
		15 P	16 S	17 Cl	18 Ar	
		33 As	34 Se	35 Br	36 Kr	
			52 Te	53 I	54 Xe	

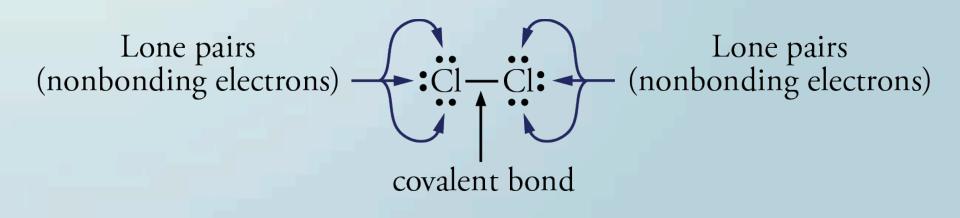
Electron-Dot Symbols and Lewis Structures

- Electron-dot symbols show valence electrons.
- or •Cl• or •Cl• or •Cl•
- Nonbonding pairs of valence electrons are called *lone pairs*.

100

Lewis Structures

 Lewis structures represent molecules using element symbols, lines for bonds, and dots for lone pairs.



Most Common Bonding Patterns for Nonmetals

Element	# Bonds	# lone pairs	
н	1	0	
С	4	0	
N, P	3	1	
O, S, Se	2	2	
F, CI, Br, I	1	3	

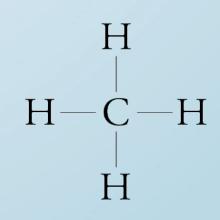
Drawing Lewis Structures

 Many Lewis structures can be drawn by attempting to give each atom in a molecule its most common bonding pattern.



Lewis Structure for Methane, CH₄

- Carbon atoms usually have 4 bonds and no lone pairs.
- Hydrogen atoms have 1 bond and no lone pairs.

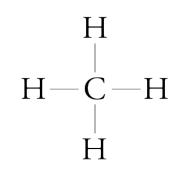


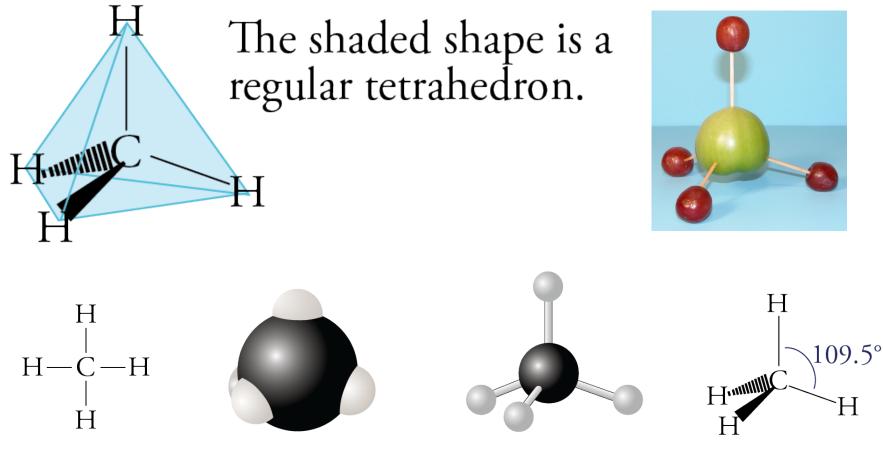
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Methane, CH₄





Lewis structure

Space-filling model

Ball-and-stick model

Geometric Sketch

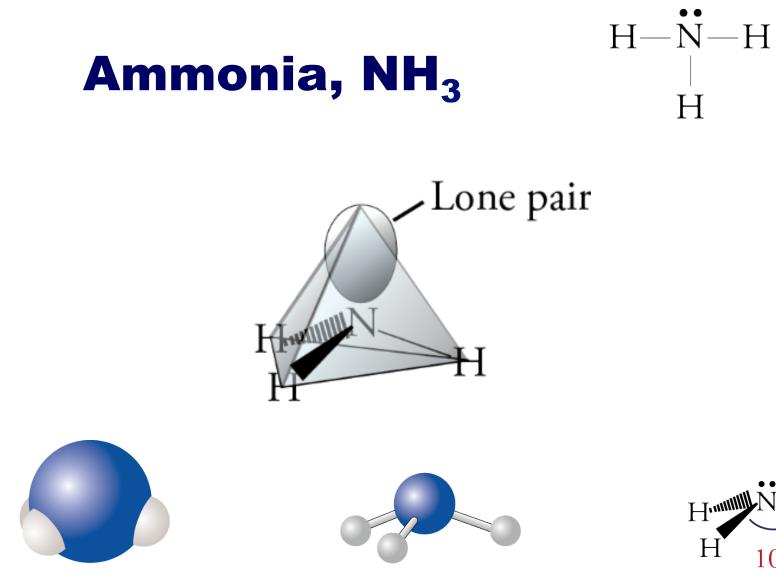
Lewis Structure for Ammonia, NH₃

- Nitrogen atoms usually have 3 bonds and 1 lone pair.
- Hydrogen atoms have 1 bond and no lone pairs.

H - N - H

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Space-filling model

Ball-and-stick model

Geometric sketch

107°

Н

Lewis Structure for Water, H₂O

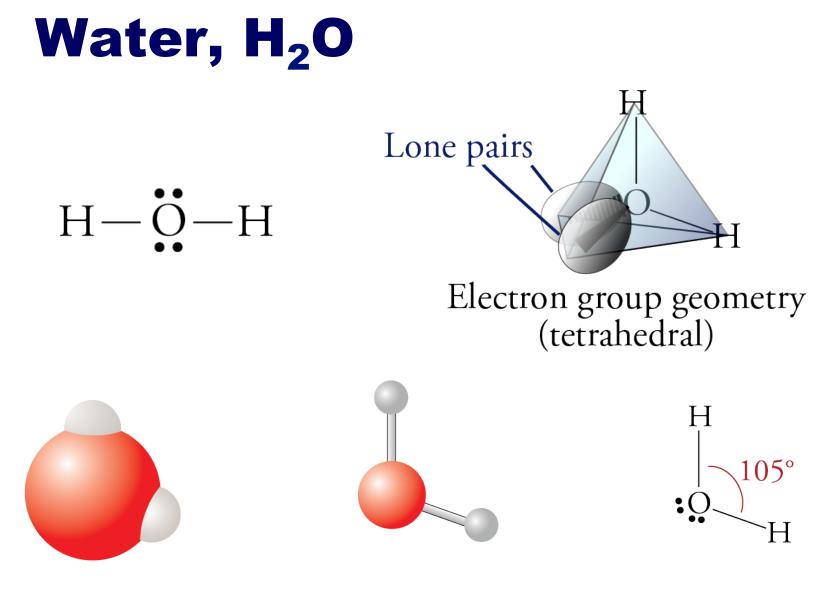
- Oxygen atoms usually have 2 bonds and 2 lone pairs.
- Hydrogen atoms have 1 bond and no lone pairs.

H - O - H

300

-200

100



Space-filling model

Ball-and-stick model

Geometric Sketch

Unique Properties of Water, H₂O

- Solid less dense than liquid (maximum density at 4 °C).
- Relatively high melting point (0 °C) and boiling point (100 °C)
- High specific heat (4.184 kJ/kg°C)

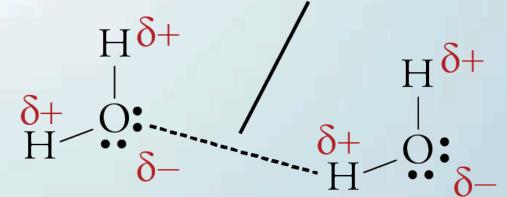
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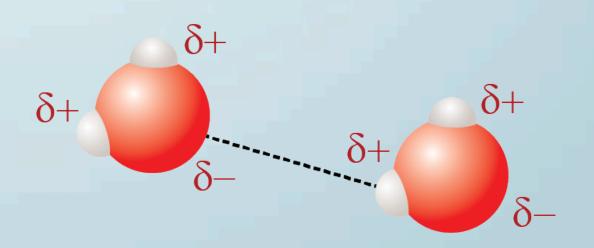
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High heat of vaporization (2258 kJ/kg)

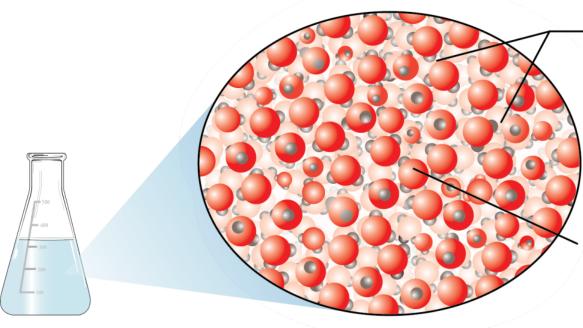
Water Attractions

Attraction between partial positive charge and partial negative charge





Liquid Water

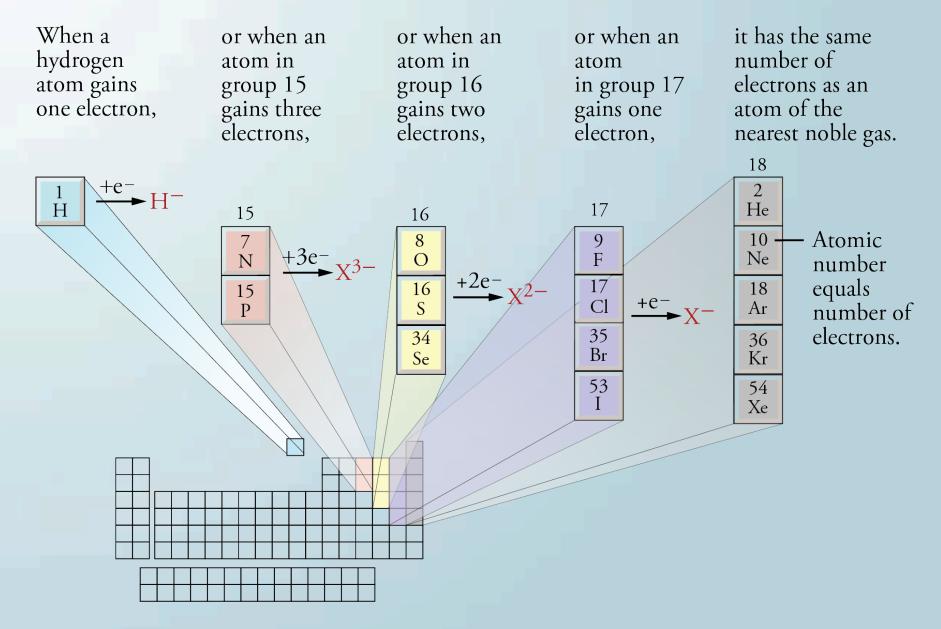


Attractions exist between hydrogen and oxygen atoms of different water molecules.

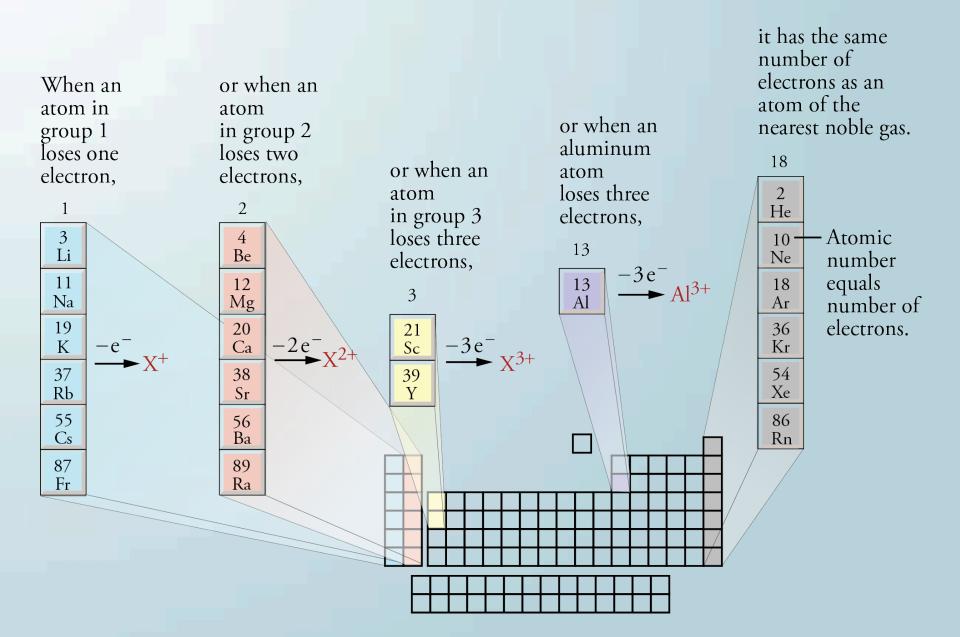
Molecules break old attractions and make new ones as they tumble throughout the liquid.

http://preparatorychemistry.com/water_flash.htm

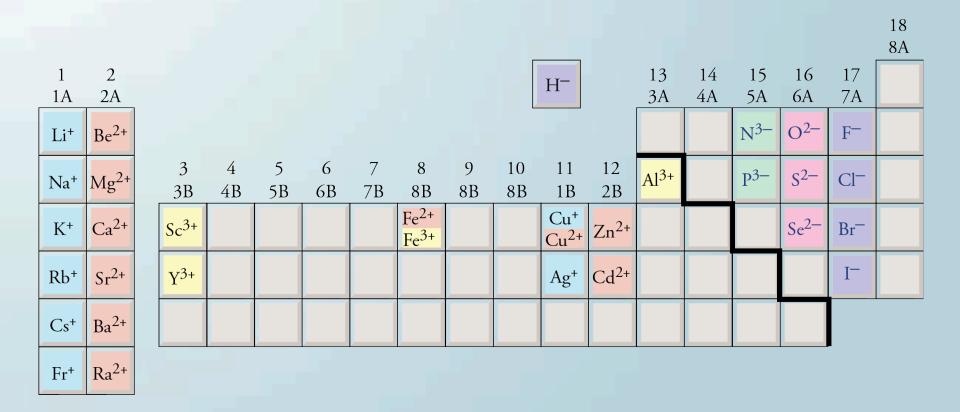
The Making of an Anion



The Making of a Cation



Monatomic Ions



Monatomic Ion Names

- Monatomic Cations
 - (name of metal)
 - Groups 1, 2, and 3 metals
 - Al³⁺, Zn²⁺, Cd²⁺, Ag⁺
 - (name of metal)(Roman numeral)
 - All metallic cations not mentioned above
- Monatomic Anions

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- (root of nonmetal name)ide

Monatomic Anions

Hydride H⁻ Nitride N³⁻ Phosphide P³⁻ Oxide O²⁻ Sulfide S²⁻ fluoride F⁻ chloride Cl⁻

bromide Br-

iodide I-

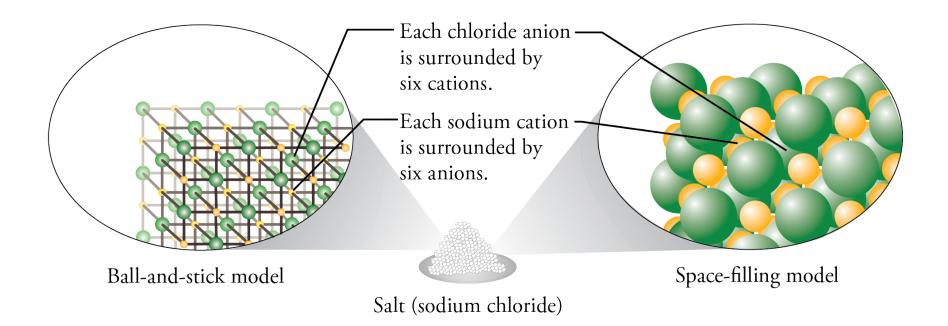
selenide Se^{2–}

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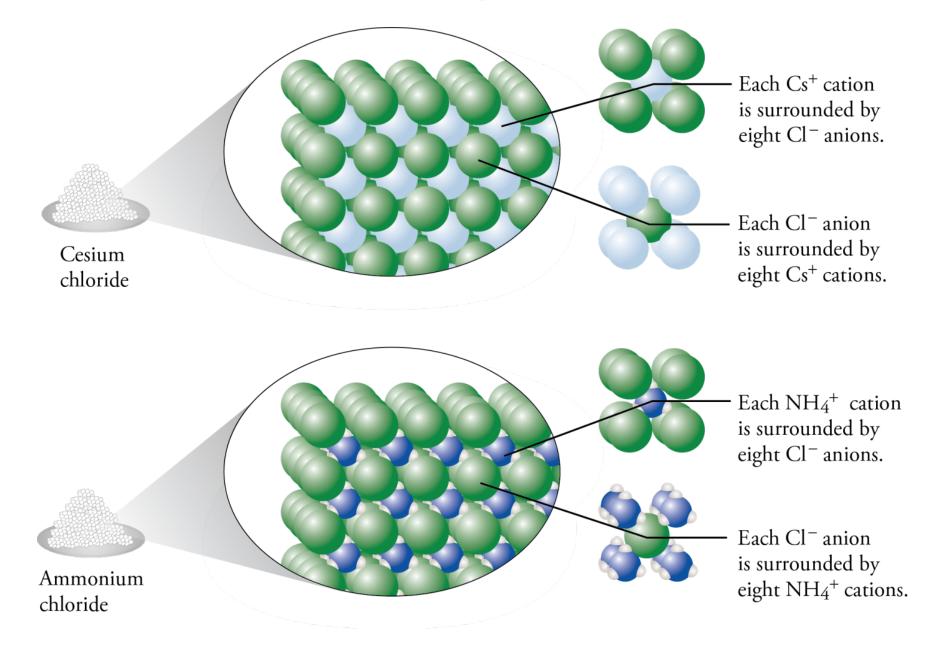
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Sodium Chloride, NaCl, Structure



CsCl and NH₄Cl structure



Polyatomic Ions

lon	Name	lon	Name
NH ₄ ⁺	ammonium	NO ₃ -	nitrate
OH⁻	hydroxide	SO ₄ ²⁻	sulfate
CO ₃ ²⁻	carbonate	$C_2H_3O_2^-$	acetate
PO ₄ ³⁻	phosphate		

Ammonium Nitrate, NH₄NO₃

- It is widely used to make fertilizers and explosives.
- Made from nitric acid and ammonia.

 $HNO_3(aq) + NH_3(g) \rightarrow NH_4NO_3(aq)$

- Not very explosive itself
- It makes an explosive mixture with hydrocarbons found in petroleum products, such as diesel fuel or kerosene.

Oklahoma City Bombing

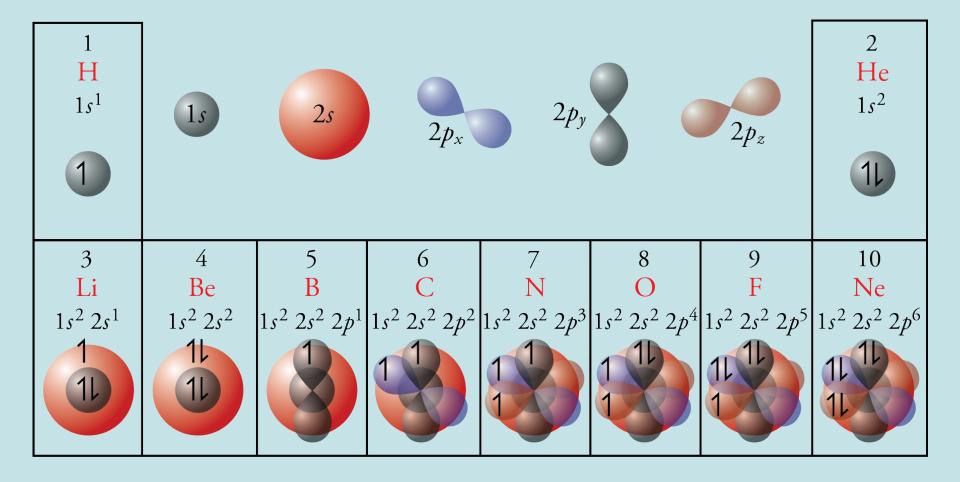
- April 19, 1995 Timothy McVeigh and Terry Nichols loaded 108 50-lb (23-kg) bags of ammonium nitrate fertilizer, three 55-U.S.-gallon (210 L) drums of liquid nitromethane, CH₃NO₂, several crates of the explosive Tovex (NH₄NO₃ and CH₃NH₃NO₃), seventeen bags of ANFO (ammonium nitrate-fuel oil), fuses, and detonators into a Ryder rental truck.
- Worst terrorist attack in U.S. until 9/11/01.
- Killed 168 people, including 19 children under the age of 6, and injured more than 680 people.

Assumptions of the Valence-Bond Model for Covalent Bonding

- Only the highest energy electrons participate in bonding.
- Covalent bonds usually form to pair unpaired electrons.

Electrons and Orbitals

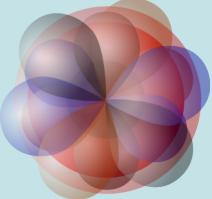
 Electrons in atoms are arranged in different energy levels, sublevels, and orbitals. (See Sections 4.2 and 4.3 in Chapter 4 of An Introduction to Chemistry – Atoms First)



Chlorine's 17 Electrons

 They are arranged in different energy levels, sublevels, and orbitals. (See Chapter 4 of An Introduction to Chemistry – Atoms First)

$$3s \stackrel{\uparrow\downarrow}{\longrightarrow} 3p \stackrel{\uparrow\downarrow}{\longrightarrow} \stackrel{\uparrow\downarrow}{\longrightarrow} \stackrel{\uparrow}{\longrightarrow}$$
$$2s \stackrel{\uparrow\downarrow}{\longrightarrow} 2p \stackrel{\uparrow\downarrow}{\longrightarrow} \stackrel{\uparrow\downarrow}{\longrightarrow} \stackrel{\uparrow\downarrow}{\longrightarrow}$$
$$1s \stackrel{\uparrow\downarrow}{\longrightarrow}$$

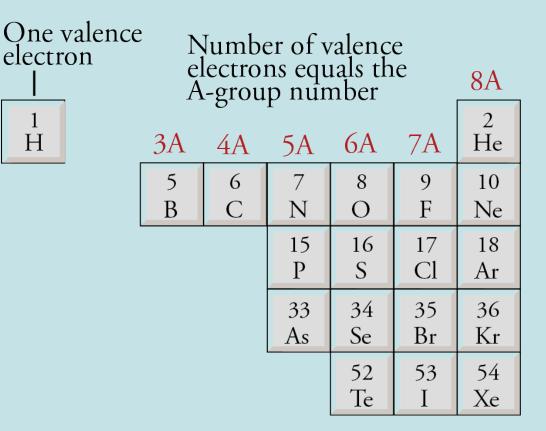


 The seven highest energy electrons have the greatest effect on the chemistry of chlorine. They are called valence electrons. They can be described with an electron dot symbol.

$$3s \downarrow 3p \downarrow \uparrow \uparrow \uparrow \uparrow ; ;;$$

Valence Electrons

- The valence electrons for each atom are the most important electrons in the formation of chemical bonds.
- The number of valence electrons for the atoms of each element is equal to the element's A-group number on the periodic table.



Chlorine, Cl₂

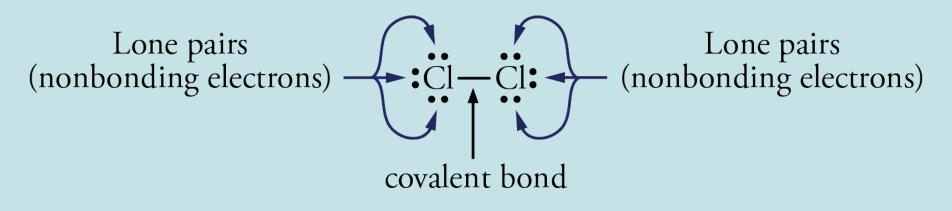
 Electron-dot symbols show valence electrons. Cl is in group 7A, so it has 7 valence electrons, leading to 7 dots spread out on the four sides of the symbol.

- Nonbonding pairs of valence electrons are called *lone pairs*.
- The unpaired electrons for each of two chlorine atoms pair to form one covalent bond.

$$\operatorname{Cl} \xrightarrow{} \operatorname{Cl} \xrightarrow{} \operatorname{Cl} \xrightarrow{} \operatorname{Cl} \operatorname{Cl} \xrightarrow{}$$

Lewis Structures

- Lewis structures represent molecules using element symbols, lines for bonds, and dots for lone pairs.
- The halogens, including chlorine, usually form one covalent bond and three lone pairs. When pure, they are composed of diatomic molecules. For example, chlorine is Cl₂.



1899 International Peace Conference

- At The Hague, Netherlands (now one of the major cities hosting the UN, along with New York and Geneva)
- 26 countries, including Germany, signed the treaty
- One section outlawed the use of "projectiles the object of which is the diffusion of asphyxiating or deleterious gases."

Chlorine and WWI

During peace time a scientist belongs to the world, but during war time he belongs to his country.



Fritz Haber

- In 1914-15, WWI, which was expected to end quickly, was bogged down in trench warfare, so each side was looking for ways to break through the lines.
- Germans thought that they could avoid violating the Hague Convention by putting poison gas and shrapnel in projectiles, based on the interpretation that the convention banned "projectiles, the sole object of which is the diffusion of asphyxiating or deleterious gases.")

- Fritz Haber, who won the Nobel Prize for chemistry in 1918, suggested loading projectiles with chlorine and shrapnel.
- Shortage of artillery shells led to use of chlorine from pressurized gas cylinders.
- Used against French near Ypres, Belgium, April 22, 1915.
- Wind conditions had to be in the correct direction, strong enough to move the gas to the enemy lines, but not too strong to disperse the gas too quickly.



Reluctance Overcome by Perceived Necessity

I must confess that the commission for poisoning the enemy, just as one poisons rats, struck me as it must any other straightforward soldier; it was repulsive to me. If, however, the poison gas were to result in the fall of Ypres, we would win a victory that might decide the entire campaign. In the view of this worthy goal, all personal reservations had to be silent. So onward, do what must be done. War is necessity and knows no exception.

Berthold von Deimling

Commander of the German XV Army Corps at Ypres



 Reacts with water to form hydrochloric acid and hypochlorous acid, which damage tissues in the lungs and draw water into the lungs.

 $CI_2 + H_2O \rightarrow HCI + HCIO$

- 168 metric tons (megagrams) released from 5730 cylinders
- Cl₂ is more dense than air
- 5-ft cloud moved at 4 mph
- Warmed, expanded to 30-ft yellow-green cloud, causing blindness, coughing, nausea, headache, and chest pain
- Created 4-mile gap in Allied line

- 600 French and Algerian troops lay blinded and dying.
- Fluid entering the lungs caused men to drown on dry land.
- Within an hour after the clearing of the gas, the Germans captured two villages, took 2000 prisoners, and confiscated 51 artillery pieces.
- German High Command had not expected the attack to work, so they did not place enough troops in the area to exploit the break in the lines, so Ypres remained in Allied hands.
- German press hailed the new innovation, but in other parts of Europe, the use of chlorine gas was condemned.

Personal Protection (Military)





Chlorine Bombs in Iraq War

- Used by insurgents against the local population and coalition forces.
- The explosion of the bombs was responsible for most of the deaths because the blast dispersed the chlorine too quickly.

Industrial Production of Chlorine

• Electrolysis of sodium chloride (table salt) in water

 $2NaCl(aq) + 2H_2O(I)$ $\rightarrow Cl_2(g) + H_2(g) + 2NaOH(aq)$

Chlorine, Cl₂, is still a Threat today.

- The United States produces approximately 1 billion pounds of chlorine a year for use in water treatment facilities.
- Potential vulnerability of chlorine-filled rail tank cars, by which chlorine is primarily transported (accident, sabotage)



Chlorine rail-car derailment, South Carolina, 2005

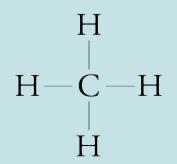
Drawing Lewis Structures from Formulas

 Most Lewis structures can be drawn by trying to arrange the atoms to get the most common bonding patterns.

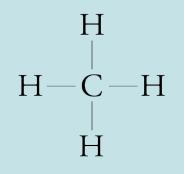
Element	# Bonds	# lone pairs
Н	1	0
С	4	0
N, P	3	1
O, S, Se	2	2
F, CI, Br, I	1	3

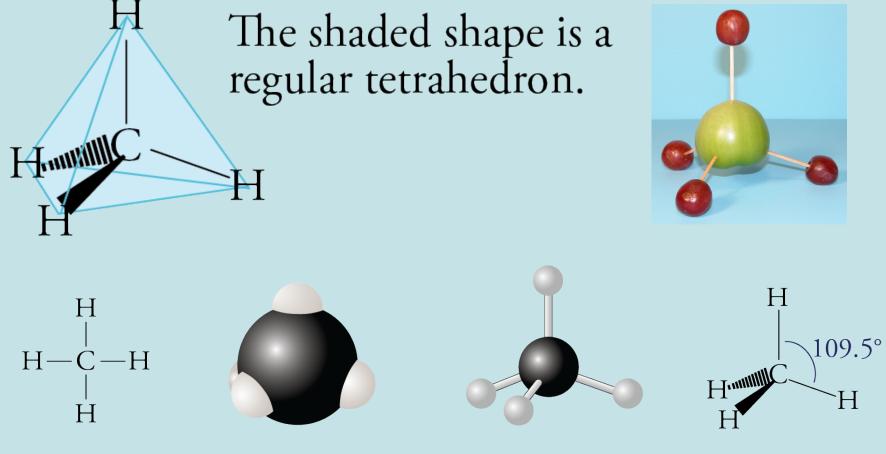
Compounds with Carbon and Hydrogen

- Compounds containing only carbon and hydrogen are called **hydrocarbons**.
- The simplest of the hydrocarbons is methane, CH₄.
- We can draw a Lewis structure for CH₄ by arranging the atoms to give the carbon atoms four bonds and the hydrogen atoms one bond.



Methane, CH₄





Lewis structure

Space-filling model

Ball-and-stick model

Geometric Sketch

Carbon – Multiple Bonds

Carbon atoms can have double or triple bonds.
 For example, ethene (ethylene), C₂H₄, has a double bond.

$$H - C = C - H$$

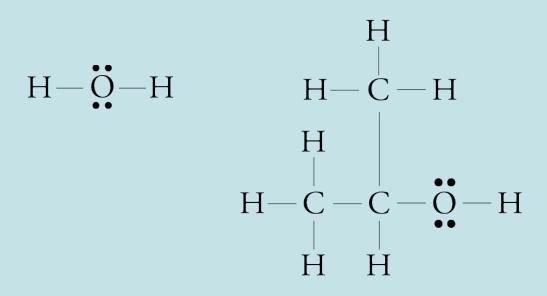
 $H H$

• Ethyne (acetylene), C_2H_2 , has a triple bond.

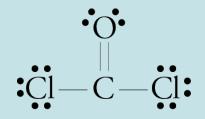
$$\mathbf{H} - \mathbf{C} \equiv \mathbf{C} - \mathbf{H}$$

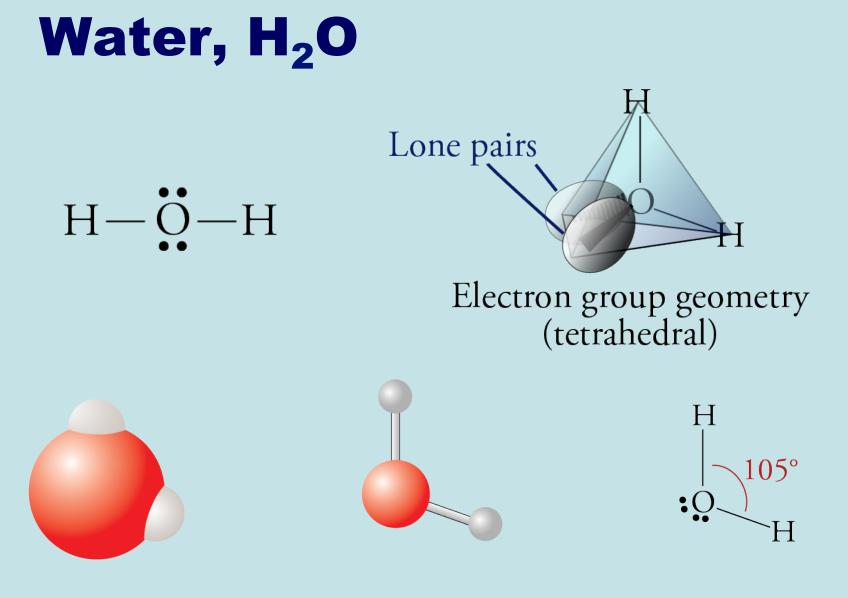
Compounds with Oxygen

 Oxygen atoms usually form two bonds and two lone pairs. For example, oxygen has two bonds and two lone pairs in water, H₂O, and in alcohols, such as 2propanol (isopropyl alcohol), CH₃CH(OH)CH₃, which is used to make the nerve gas sarin.



 Oxygen atoms often form double bonds, e.g. in the chemical weapon phosgene, COCl₂.

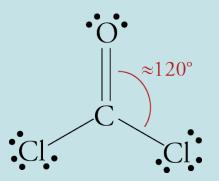




Space-filling model

Ball-and-stick model

Geometric Sketch

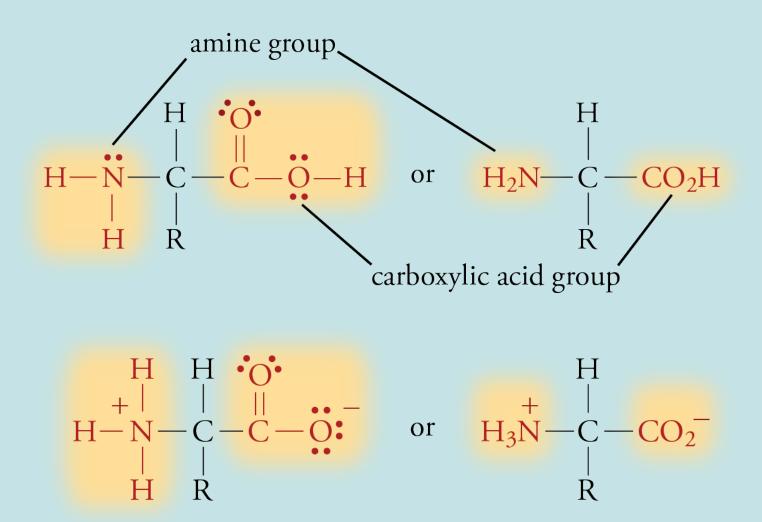


• Produced from carbon monoxide and chlorine. $CO + Cl_2 \rightarrow COCl_2$

Phosgene, **COCl**₂

- 18 times more toxic than Cl₂
- It causes suffocation by reacting with proteins in the lungs to disrupt the blood-air barrier.
- Smells like new-mown hay
- Less irritating than Cl₂, so soldiers were slower to put on their gas masks
- In December 1915, the Germans fired shells containing phosgene gas, and the French retaliated in February 1916.

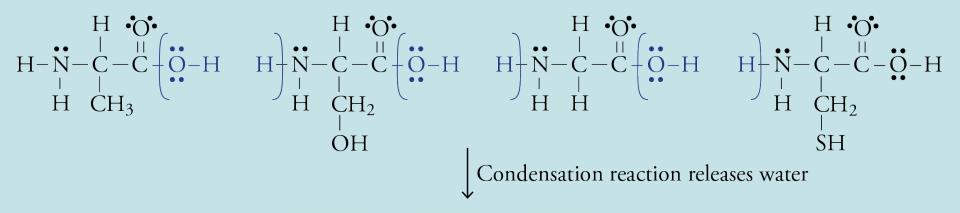
Amino Acids

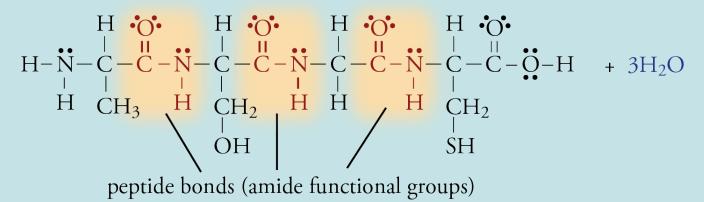




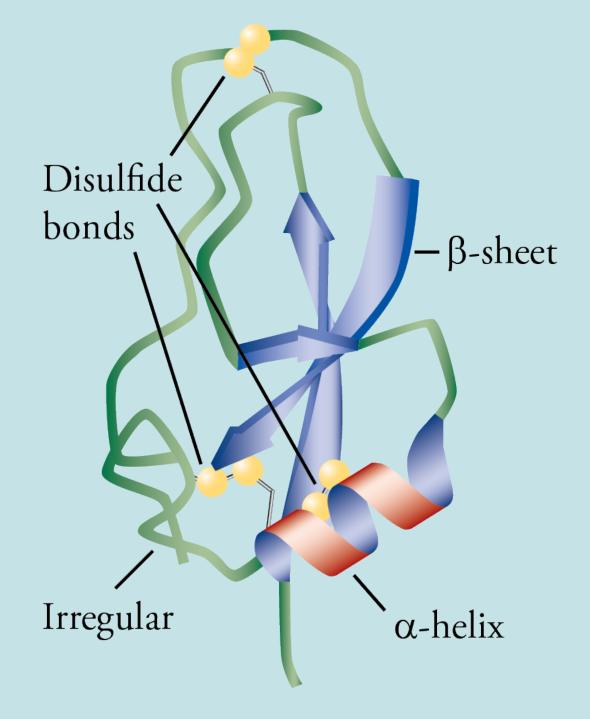
Η $\begin{array}{c}
\oplus \\
H_3N - C - CO_2^{\ominus}
\end{array}$ CH_2 CH₂ CH_2 CH_2 NH_2

Formation of Ala-Ser-Gly-Cys



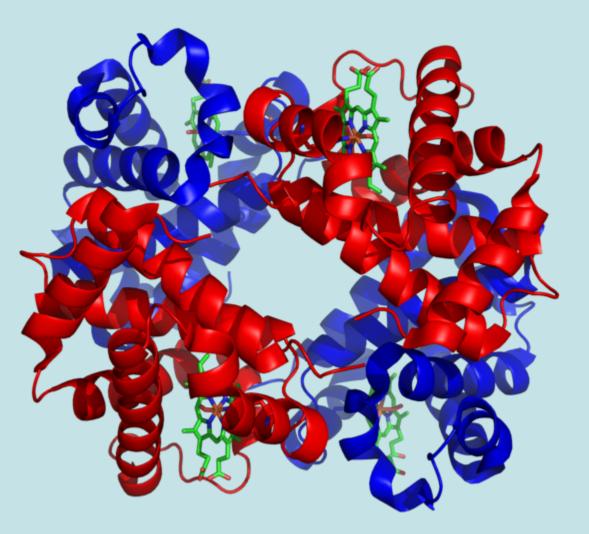


The Ribbon Structure of the Protein BPTI



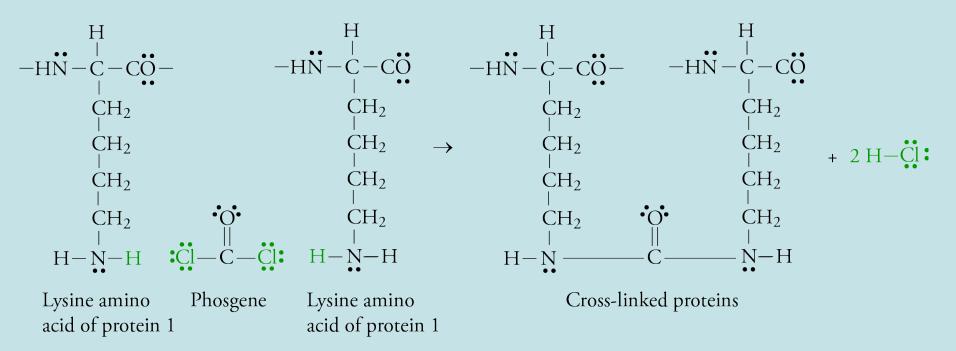
Hemoglobin

 The protein hemoglobin carries oxygen in the blood.



Phosgene Reaction with Protein

- Phosgene reacts with proteins in the lungs to disrupt the blood-air barrier, causing suffocation.
- It reacts with the amines of the proteins, linking protein together
- The cross-linked proteins no longer function in their normal way.

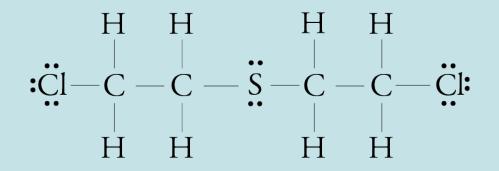


Dual Use

- A small-scale malicious chemical program can easily be hid behind a normal industrial/research chemistry front.
 - Chlorine is used for water purification and to make many other compounds.
 - Phosgene is used to make important compounds, including pharmaceuticals and plastics.

Compounds with Sulfur

 Sulfur atoms usually form two bonds and two lone pairs. For example, sulfur has two bonds and two lone pairs in the mustard agent CICH₂CH₂SCH₂CH₂CI.



Compounds with Nitrogen

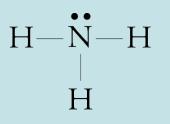
 Nitrogen atoms usually form three bonds and one lone pair. For example, nitrogen has three bonds and one lone pair in ammonia, NH₃, and hydrogen cyanide, HCN, (a blood agent).

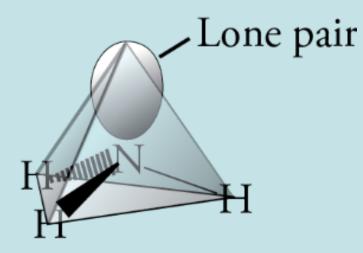
$$\begin{array}{ccc} H - \stackrel{\bullet \bullet}{N} - H & H - C \equiv N \\ & H \\ H \end{array}$$

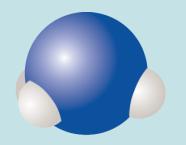
 Nitrogen has four bonds and one lone pair in the ammonium polyatomic ion, NH₄⁺.

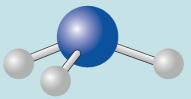
$$\begin{bmatrix} H \\ | \\ H - N - H \\ | \\ H \end{bmatrix}$$













Space-filling model

Ball-and-stick model

Geometric sketch

Ammonia and Chemical Explosives

- Fritz Haber figured out a way to make ammonia, NH₃, from N₂ in the air. This was difficult because the bond between nitrogen atoms in N₂ is very strong and difficult to break. N₂(g) + 3H₂(g) \rightleftharpoons 2 NH₃(g)
- The NH₃ can be used to make chemical fertilizers. It can also be converted into nitric acid, which is used to make chemical explosives.

 $4\mathrm{NH}_3 + 5\mathrm{O}_2 \rightarrow 4\mathrm{NO} + 6\mathrm{H}_2\mathrm{O}$

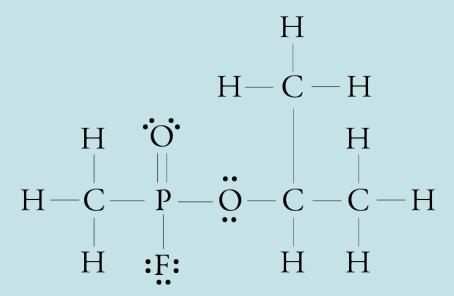
 $2NO + O_2 \rightarrow 2NO_2$

 $3NO_2 + H_2O \rightarrow 2HNO_3 + NO$

In a series of steps, nitric acid, HNO₃, reacts with glycerine to form nitroglycerine or with toluene to form trinitrotoluene (TNT). (more later)

Compounds with Phosphorus

 Phosphorus atoms usually form three bonds and one lone pair, but they can form five bonds in compounds such as the nerve gas sarin.



Polyatomic lons with Hydrogen

- HCO₃⁻ hydrogen carbonate
- HSO₄⁻ hydrogen sulfate
- HS⁻ hydrogen sulfide

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- HPO₄²⁻ hydrogen phosphate
- H₂PO₄⁻ dihydrogen phosphate

Mole

- 300

-200

-100

- A *mole* (mol) is an amount of substance that contains the same number of particles as there are atoms in 12 g of carbon-12.
- To four significant figures, there are 6.022×10^{23} atoms in 12 g of carbon-12.
- Thus a mole of natural carbon is the amount of carbon that contains 6.022×10^{23} carbon atoms.
- The number 6.022 × 10²³ is often called Avogadro's number.

Avogadro's Number



If the extremely tiny atoms in just 12 grams of carbon are arranged in the line, the line would extend over 500 times the distance between earth and the sun.

Molar Mass For Elements

200

Atomic Mass from the Periodic Table

(atomic mass) g element

Molar Mass Calculation for Carbon

$$? \operatorname{mol} C = 0.55 \operatorname{carat} C \left(\frac{1 \operatorname{g}}{5 \operatorname{carat}} \right) \left(\frac{1 \operatorname{mol} C}{12.011 \operatorname{g} C} \right) = 9.2 \times 10^{-3} \operatorname{mol} C$$

Molecular Mass

• Whole = sum of parts

300

-200

100

- mass of a molecule = sum of the masses of the atoms in the molecule
- molecular mass = the sum of the atomic masses of the atoms in the molecule

Molar mass O: 15.9994 g/mol Molar mass H: 1.00794 g/mol 1.00794 g/mol

Molar mass H₂O: 18.0153 g/mol

Molar Mass For Molecular Compounds

 Molecular Mass = Sum of the atomic masses of atoms in one molecule

100

(molecular mass) g molecular compound 1 mol molecular compound

Formula Units

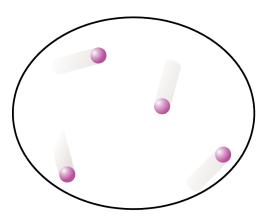
200

100

- A formula unit of a substance is the group represented by the substance's chemical formula, that is, a group containing the kinds and numbers of atoms or ions listed in the chemical formula.
- Formula unit is a general term that can be used in reference to elements, molecular compounds, or ionic compounds.

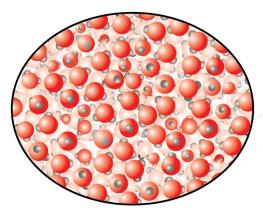
Formula Unit Examples

neon gas (element)



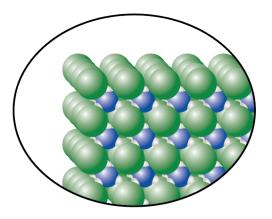
A formula unit of neon contains one Ne atom.

liquid water (molecular compound)



Liquid water is composed of discrete H₂O molecules.

A formula unit of water contains one oxygen atom and two hydrogen atoms. ammonium chloride (ionic compound)



There are no separate ammonium chloride, NH_4Cl , molecules. Each ion is equally attracted to eight others. A formula unit of ammonium chloride contains one ammonium ion, NH_4^+ , and one chloride ion, Cl^- , (or one nitrogen atom, four hydrogen atoms, and one chloride ion).



Formula Mass for Ionic Compounds

- Whole = sum of parts
- Mass of a formula unit = sum of the masses of the atoms in the formula unit
- Formula mass = the sum of the atomic masses of the atoms in the formula

Formula unit NaCl Molar mass Na: 22.9898 g/mol Molar mass Cl: 35.4527 g/mol Molar mass NaCl: 58.4425 g/mol

Molar Mass For Ionic Compounds

 Formula Mass = Sum of the atomic masses of the atoms in a formula unit

(formula mass) gionic compound 1 mol ionic compound

-200

100