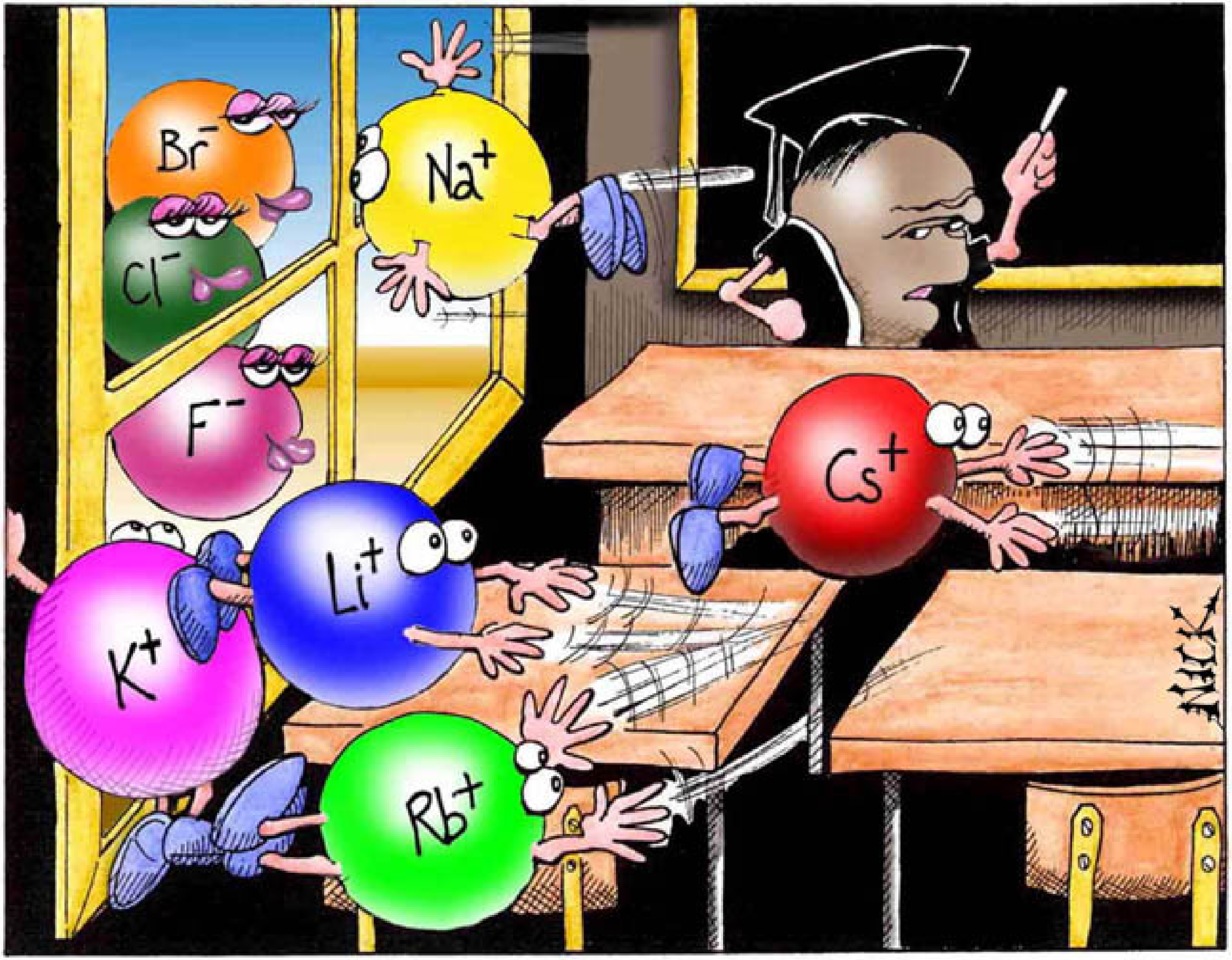
Unit 3: Chemical Bonding and Molecular Structure



"Perhaps one of you gentlemen would mind telling me just what it is outside the window that you find so attractive..?"

Cartoon courtesy of NearingZero.net

Bonds

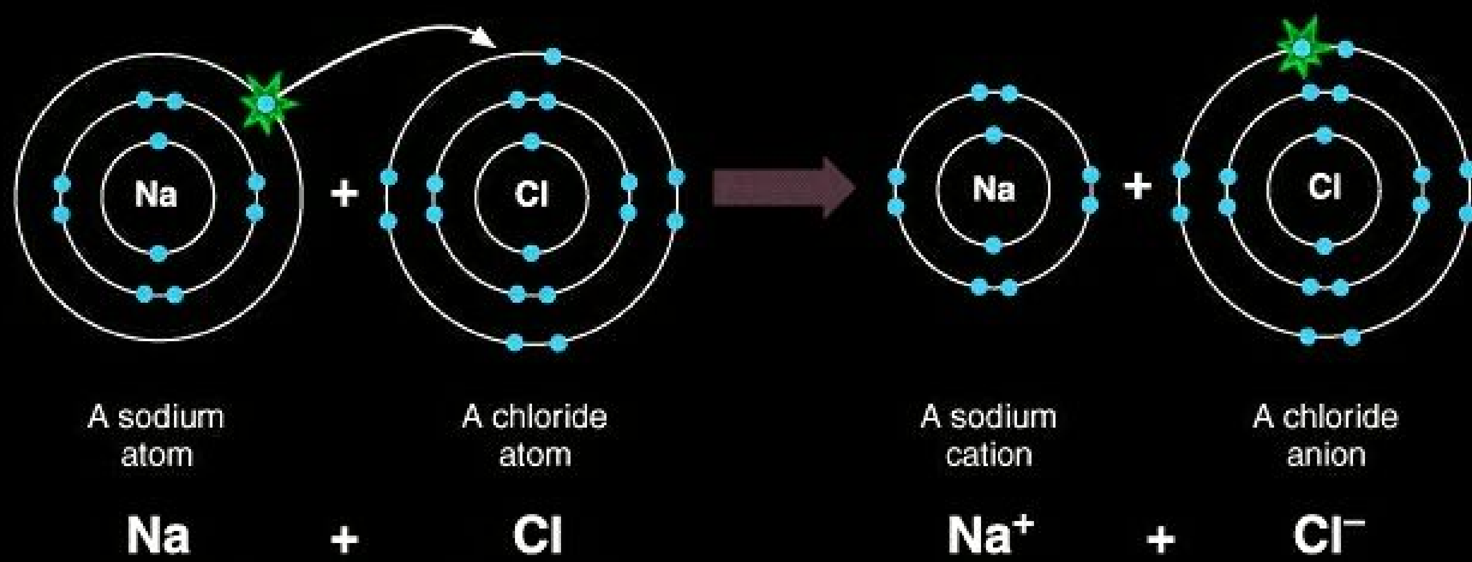
- Forces that hold groups of atoms together and make them function as a unit.
    - Ionic bonds – transfer of electrons
    - Covalent bonds – sharing of electrons

Electron Dot Notation

Element	Electron config.	Electron dot symbol
Li	[He]$2s^1$	Li
Be	[He]$2s^2$	Be
B	[He]$2s^2 2p^1$	B
C	[He]$2s^2 2p^2$	C
N	[He]$2s^2 2p^3$	N
O	[He]$2s^2 2p^4$	O
F	[He]$2s^2 2p^5$	F
Ne	[He]$2s^2 2p^6$	Ne

The Octet Rule – Ionic Compounds

Ionic compounds tend to form so that each atom, by <u>gaining or losing</u> electrons, has an octet of electrons in its highest occupied energy level.



Ionic Bonding:
The Formation of Sodium Chloride

- Sodium has 1 valence electron
- Chlorine has 7 valence electrons
- An electron transferred gives each an octet

Na $1s^2 2s^2 2p^6 \mathbf{3s^1}$

Cl $1s^2 2s^2 2p^6 3s^2 \mathbf{3p^5}$

Ionic Bonding: The Formation of Sodium Chloride

This transfer forms **ions, each with an octet**:

Na^{+} $1s^2 2s^2 2p^6$

Cl^{-} $1s^2 2s^2 2p^6 3s^2 3p^6$

Ionic Bonding:
The Formation of Sodium Chloride

The resulting ions come together due to electrostatic attraction (opposites attract):

$Na^+ Cl^-$

The net charge on the compound must equal zero

Examples of Ionic compounds

All salts, which are composed of metals bonded to nonmetals, are ionic compounds and form ionic crystals.

Examples:

$Mg^{2+}Cl^{-}_{2}$

$Na^{+}_{2}O^{2-}$

$Ca^{2+}O^{2-}$

$K^{+}I^{-}$

$Li^{+}F^{-}$

$Ba^{2+}S^{2-}$

Monatomic Cations	Name
H^{+}	Hydrogen
Li^{+}	Lithium
Na^{+}	Sodium
K^{+}	Potassium
Mg^{2+}	Magnesium
Ca^{2+}	Calcium
Ba^{2+}	Barium
Al^{3+}	Aluminum

Monatomic Anions	Name
F^-	Fluoride
Cl^-	Chloride
Br^-	Bromide
I^-	Iodide
O^{2-}	Oxide
S^{2-}	Sulfide
N^{3-}	Nitride
P^{3-}	Phosphide

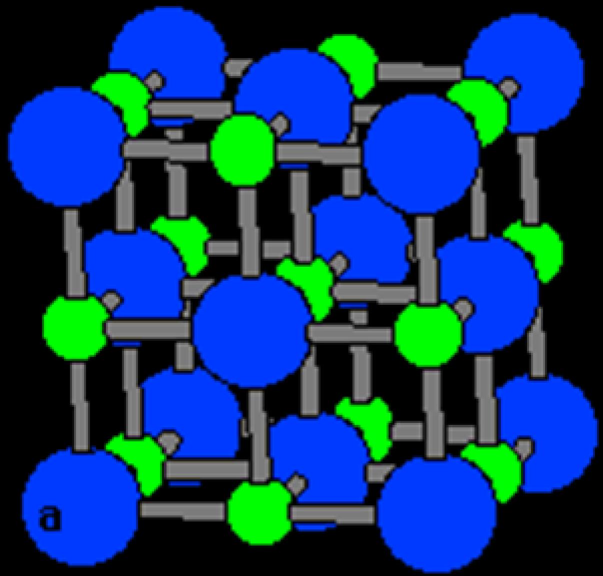
Properties of Ionic Compounds

Structure:	Crystalline solids
Melting point:	Generally high
Boiling Point:	Generally high
Electrical Conductivity:	Excellent conductors, molten and aqueous
Solubility in water:	Generally soluble

Sodium Chloride Crystal Lattice

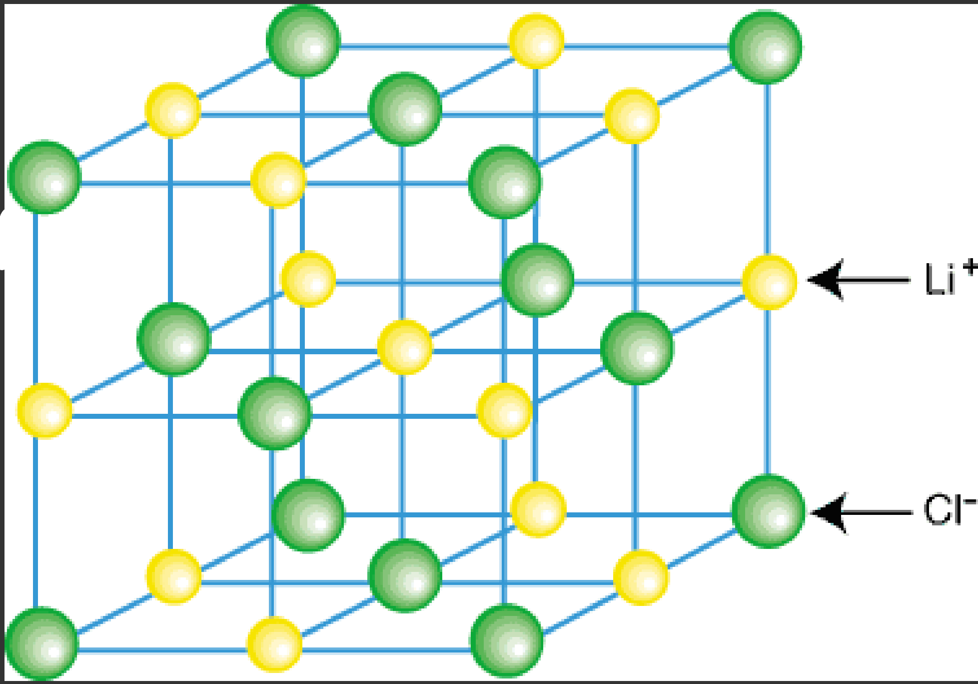
Ionic compounds form solids at ordinary temperatures.

Ionic compounds organize in a characteristic crystal lattice of alternating positive and negative ions.



Representation of Components in an Ionic Solid

Lattice: A 3-dimensional system of points designating the centers of components (atoms, ions, or molecules) that make up the substance.



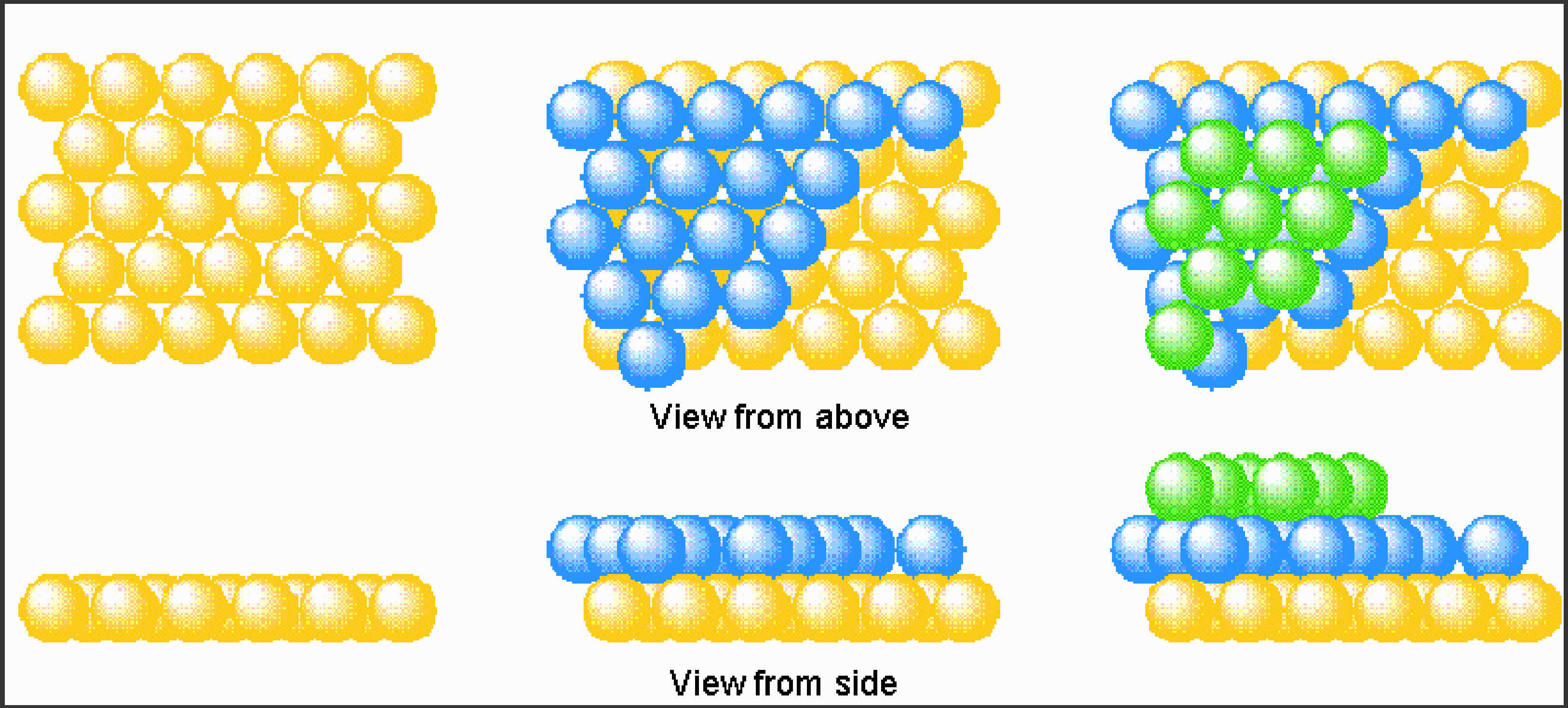
Metallic Bonding

- The chemical bonding that results from the attraction between metal atoms and the surrounding sea of electrons
- Vacant *p* and *d* orbitals in metal's outer energy levels overlap, and allow outer electrons to move freely throughout the metal
- Valence electrons do not belong to any one atom

Properties of Metals

- Metals are good conductors of heat and electricity
- Metals are malleable
- Metals are ductile
- Metals have high tensile strength
- Metals have luster

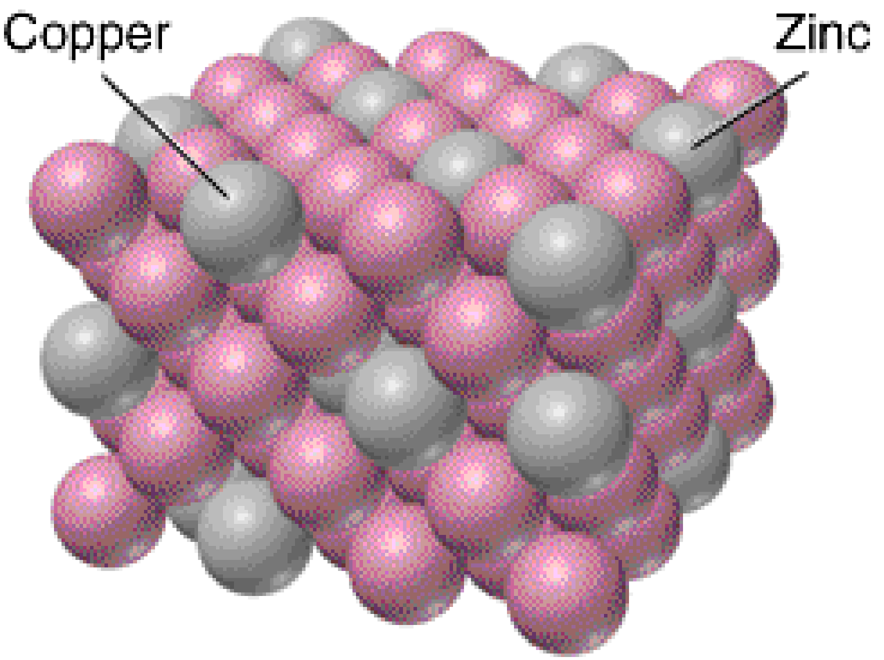
Packing in Metals



Model: Packing uniform, hard spheres to best use available space. This is called closest packing. Each atom has 12 nearest neighbors.

Metal Alloys

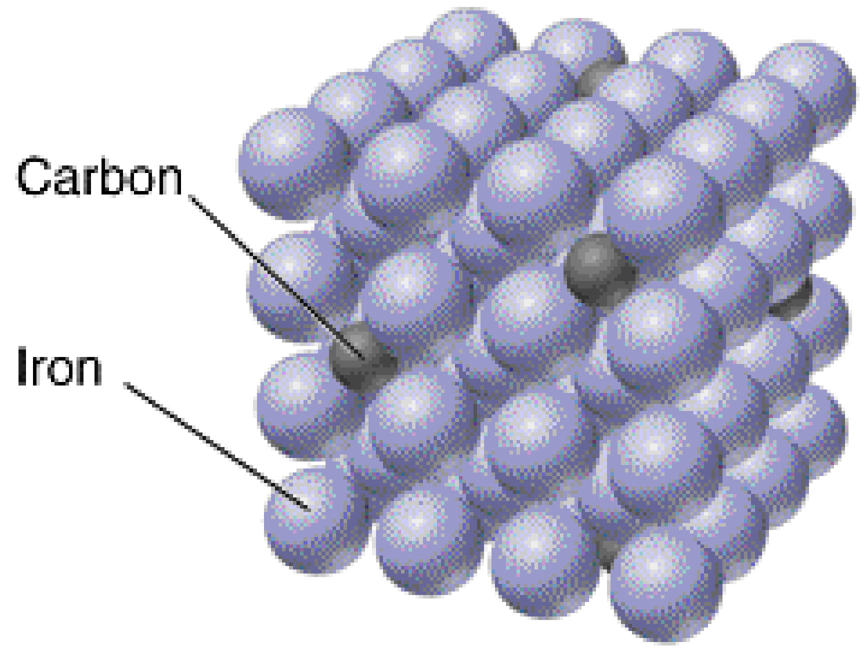
- **Substitutional Alloy**: some metal atoms **replaced** by others of similar size.



A Brass, a substitutional alloy

Metal Alloys

- **Interstitial Alloy:** Interstices (holes) in closest packed metal structure are occupied by small atoms.

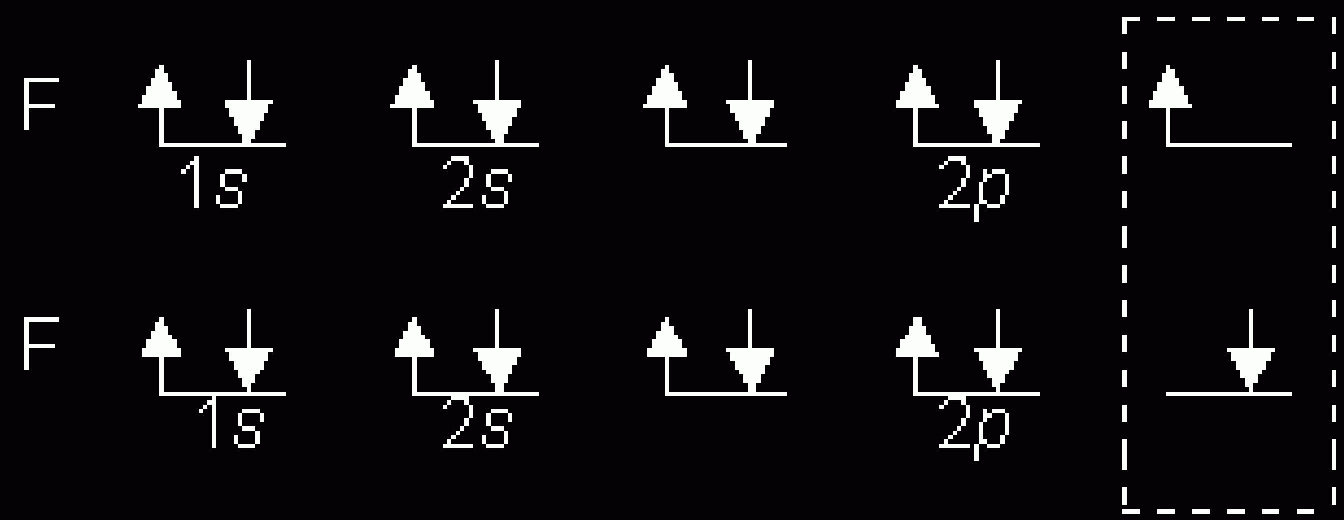


B Carbon steel, an interstitial alloy

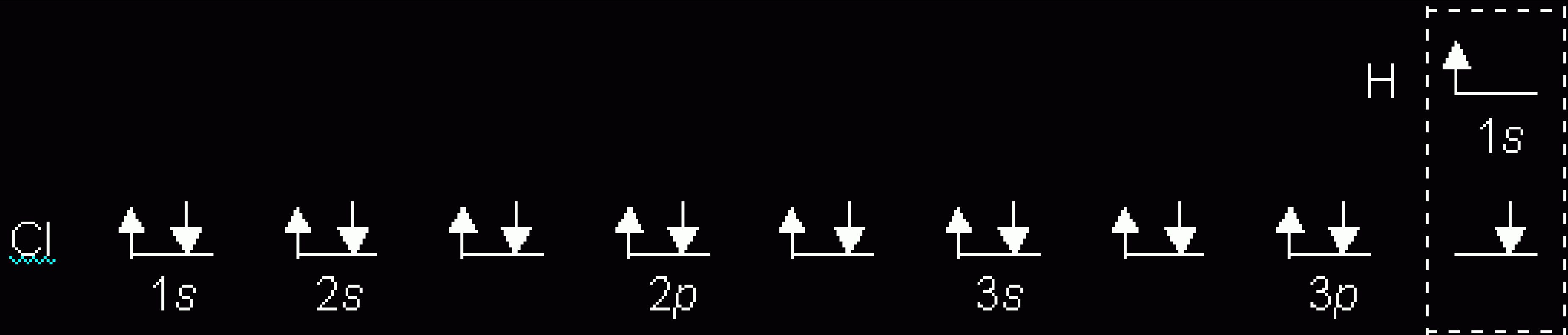
The Octet Rule – Covalent Compounds

Covalent compounds tend to form so that each atom, by sharing electrons, has an octet of electrons in its highest occupied energy level.

Diatomic Fluorine

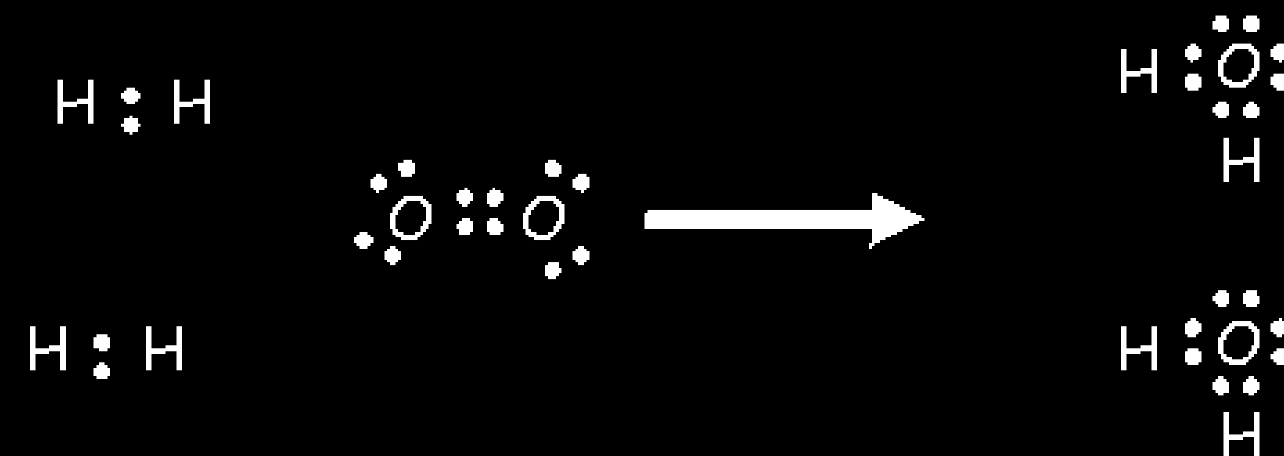


Hydrogen Chloride by the Octet Rule



Formation of Water by the Octet Rule

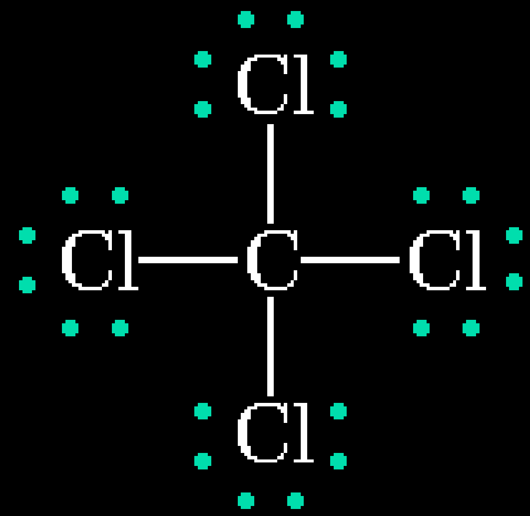
$$2H_2 + O_2 \rightarrow 2H_2O$$



Comments About the Octet Rule

- 2nd row elements C, N, O, F observe the octet rule.
- 2nd row elements B and Be often have fewer than 8 electrons around themselves - they are very reactive.
- 3rd row and heavier elements CAN exceed the octet rule using empty valence *d* orbitals.
- When writing Lewis structures, satisfy octets first, then place electrons around elements having available *d* orbitals.

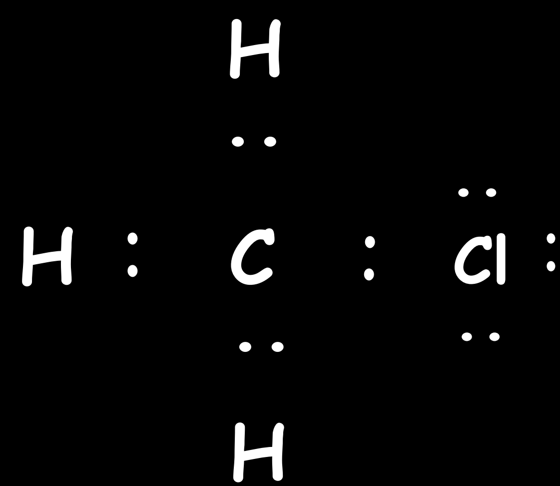
Lewis Structures



- Shows how valence electrons are arranged among atoms in a molecule.
- Reflects central idea that stability of a compound relates to noble gas electron configuration.

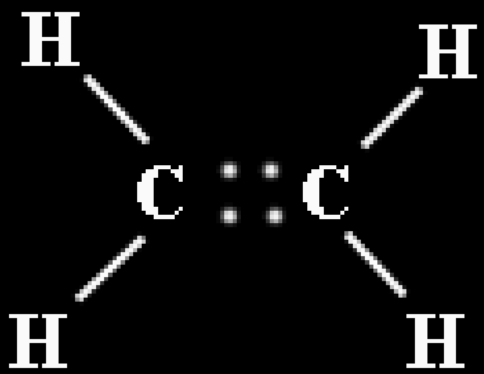
Completing a Lewis Structure -CH_3Cl

- Make carbon the central atom
- Add up available valence electrons:
  - C = 4, H = (3)(1), Cl = 7   Total = 14
- Join peripheral atoms to the central atom with electron pairs.
- Complete octets on atoms other than hydrogen with remaining electrons

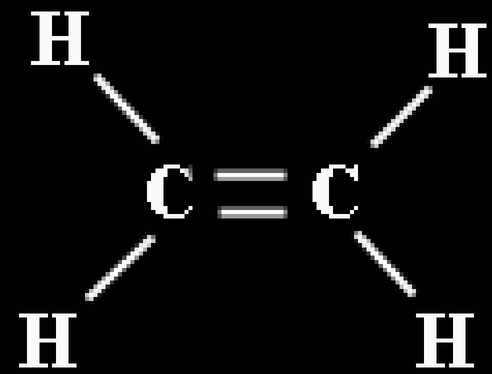


Multiple Covalent Bonds:
Double bonds

ethene



or...



Two pairs of shared electrons

Multiple Covalent Bonds:
Triple bonds

ethyne (acetylene)

$$H-C\equiv C-H$$

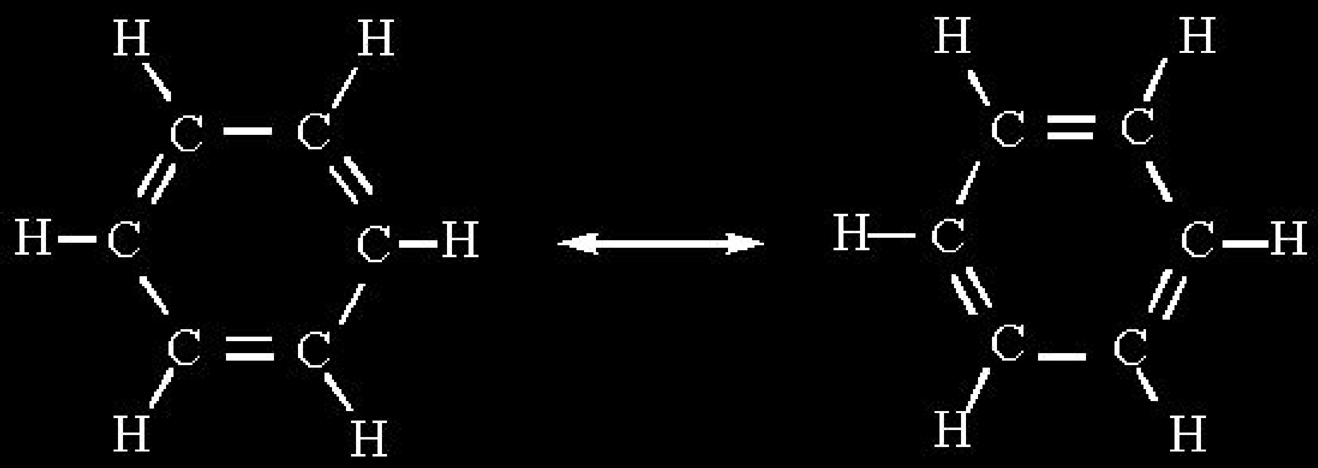
Three pairs of shared electrons

Bond Length and Bond Energy

Bond	Length (pm)	Energy (kJ/mol)
C - C	154	346
C=C	134	612
C≡C	120	835
C - N	147	305
C=N	132	615
C≡N	116	887
C - O	143	358
C=O	120	799
C≡O	113	1072
N - N	145	180
N=N	125	418
N≡N	110	942

Resonance

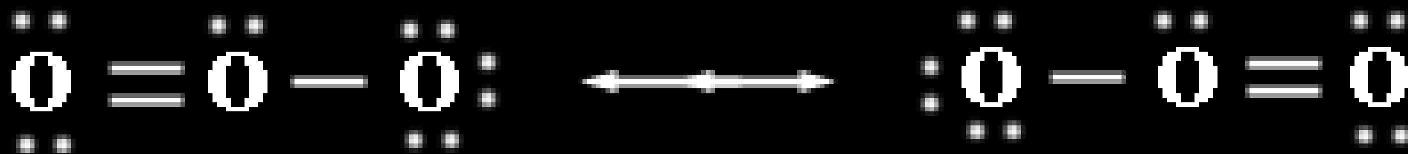
- Occurs when more than one valid Lewis structure can be written for a particular molecule.



- These are resonance structures. The actual structure is an average of the resonance structures.

Resonance in Ozone

Ozone (O_3)



Neither structure is correct.

Models

Models are attempts to explain how nature operates on the microscopic level based on experiences in the macroscopic world.

Models can be physical as with this DNA model

Models can be mathematical

Models can be theoretical or philosophical

Fundamental Properties of Models

- A model does not equal reality.
- Models are oversimplifications, and are therefore often wrong.
- Models become more complicated as they age.
- We must understand the underlying assumptions in a model so that we don't misuse it.

VSEPR Model
(Valence Shell Electron Pair Repulsion)

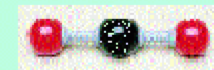
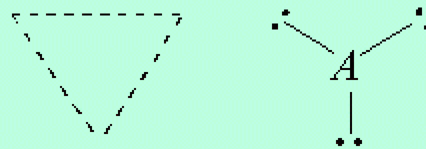
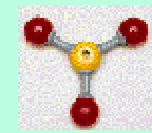
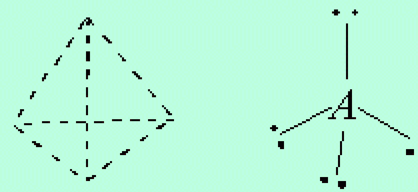
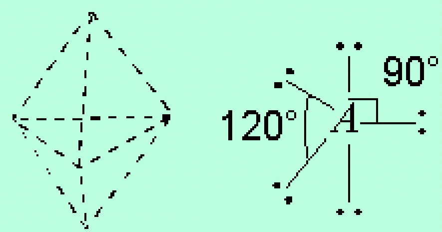
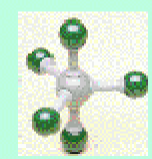
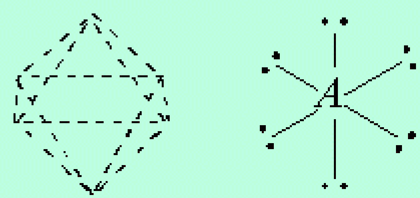
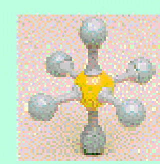
- The structure around a given atom is determined *principally* by minimizing electron pair repulsions.

Predicting a VSEPR Structure

- Draw Lewis structure.
- Put pairs as far apart as possible.
- Determine positions of atoms from the way electron pairs are shared.
- Determine the name of molecular structure from positions of the atoms.

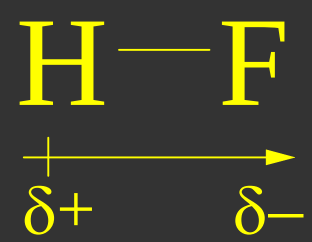
Table – VSEPR Structures

Table 8.6 Arrangements of Electron Pairs Around an Atom Yielding Minimum Repulsion

Number of Electron Pairs		Arrangement of Electron Pairs	Example
2	Linear		
3	Trigonal planar		
4	Tetrahedral		
5	Trigonal bipyramidal		
6	Octahedral		

Polarity

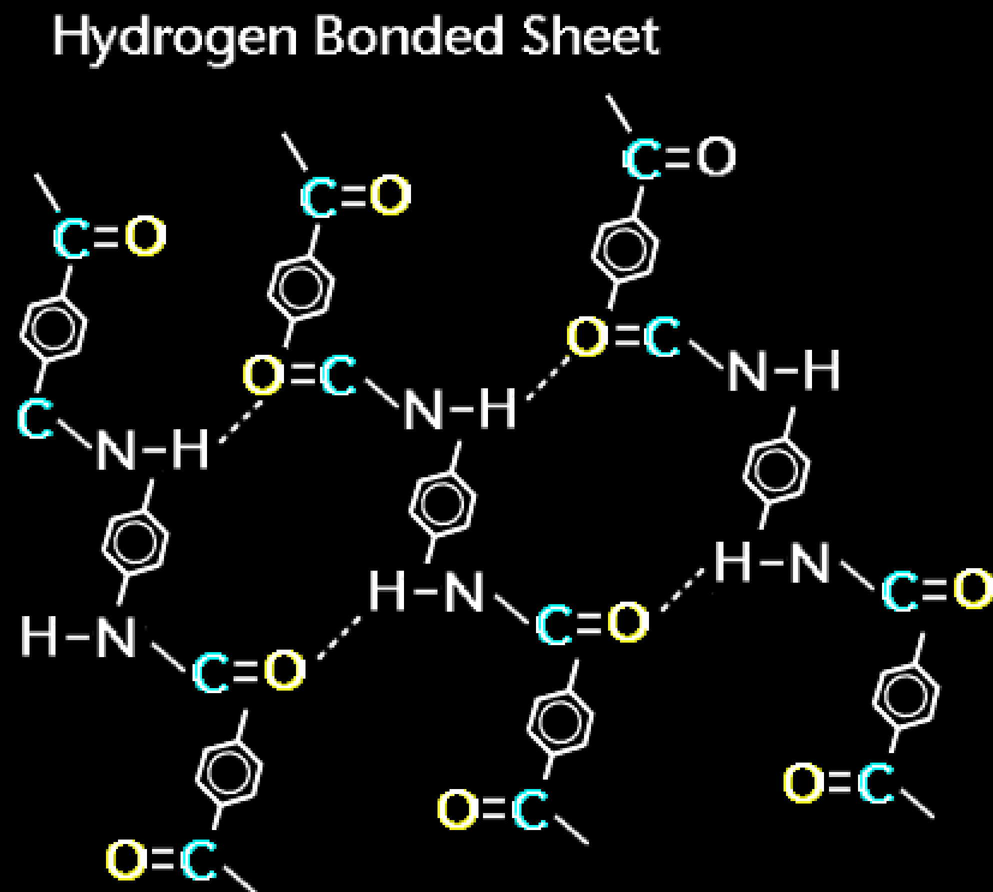
A molecule, such as HF, that has a center of positive charge and a center of negative charge is said to be polar, or to have a dipole moment.



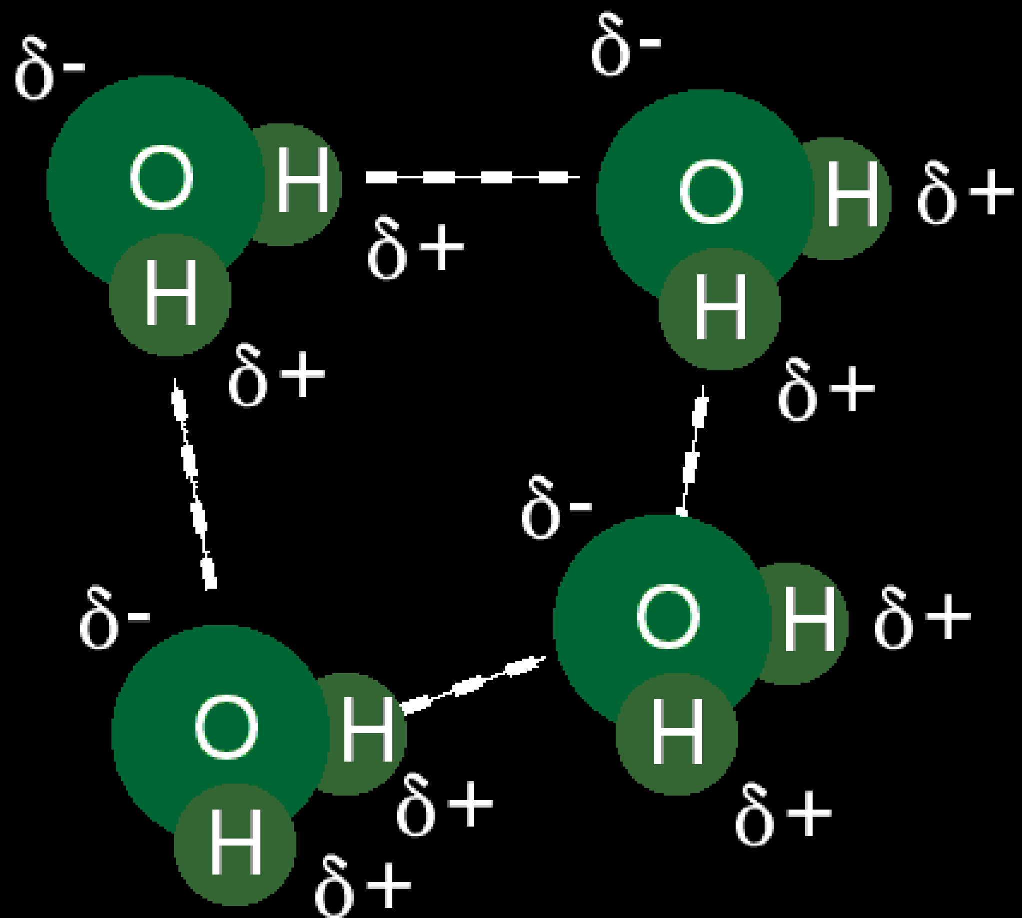
Hydrogen Bonding

Bonding between hydrogen and more electronegative neighboring atoms such as oxygen and nitrogen

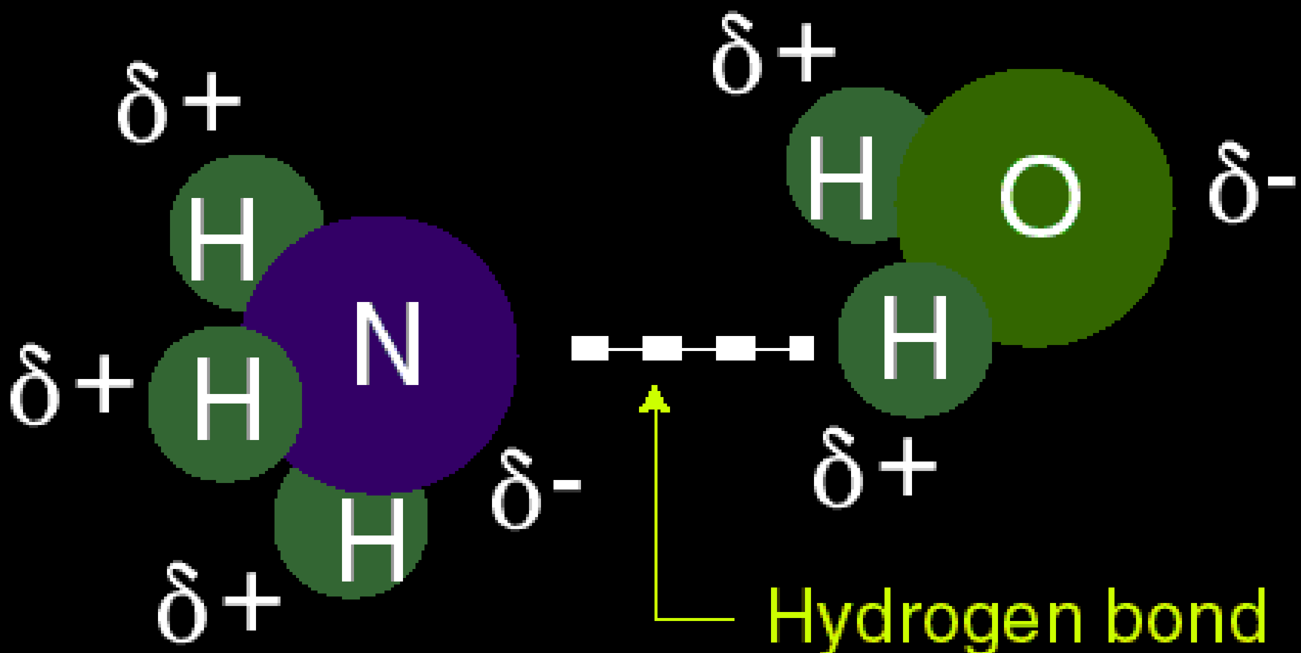
Hydrogen bonding in Kevlar, a strong polymer used in bullet-proof vests.



Hydrogen Bonding in Water

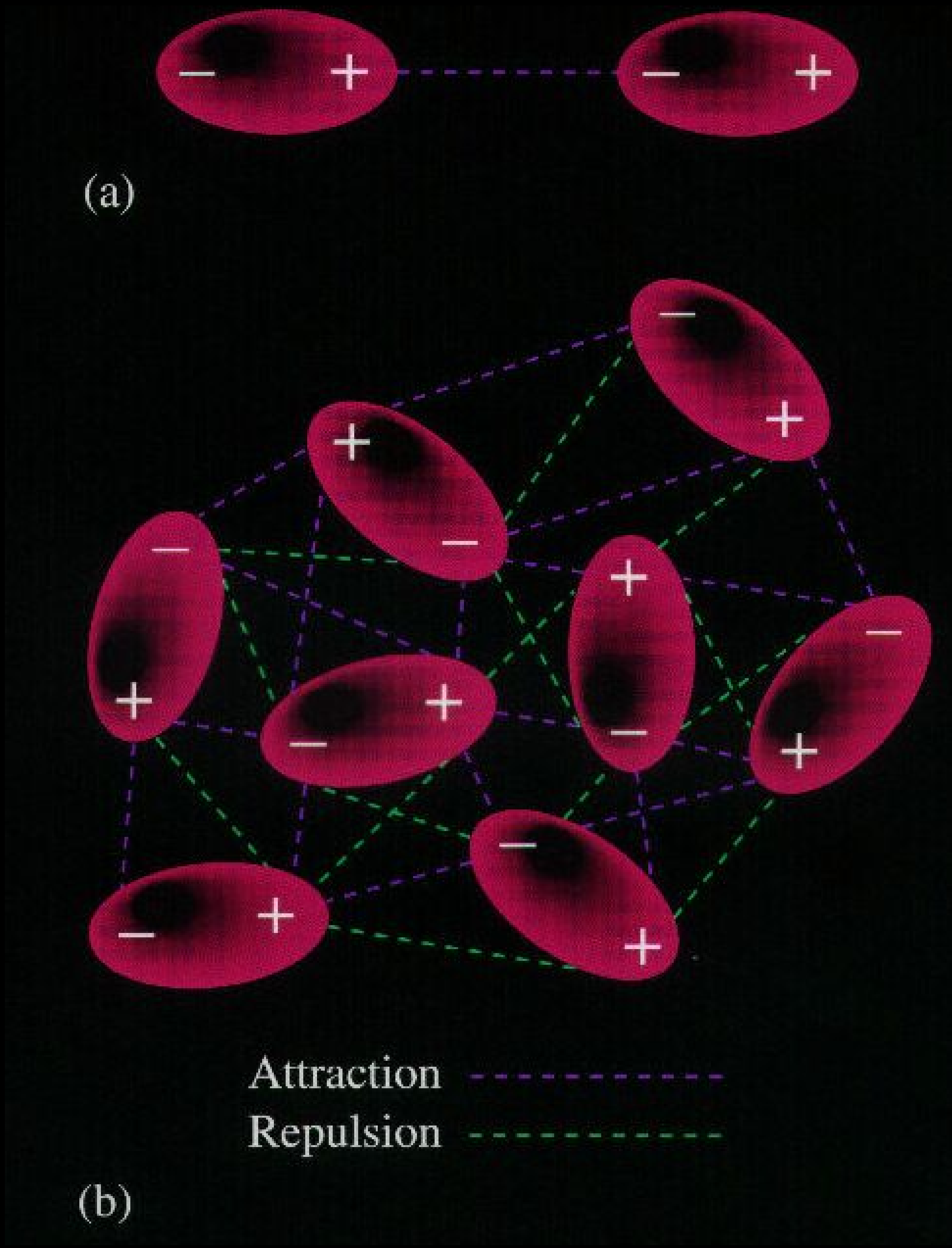


Hydrogen Bonding between Ammonia and Water

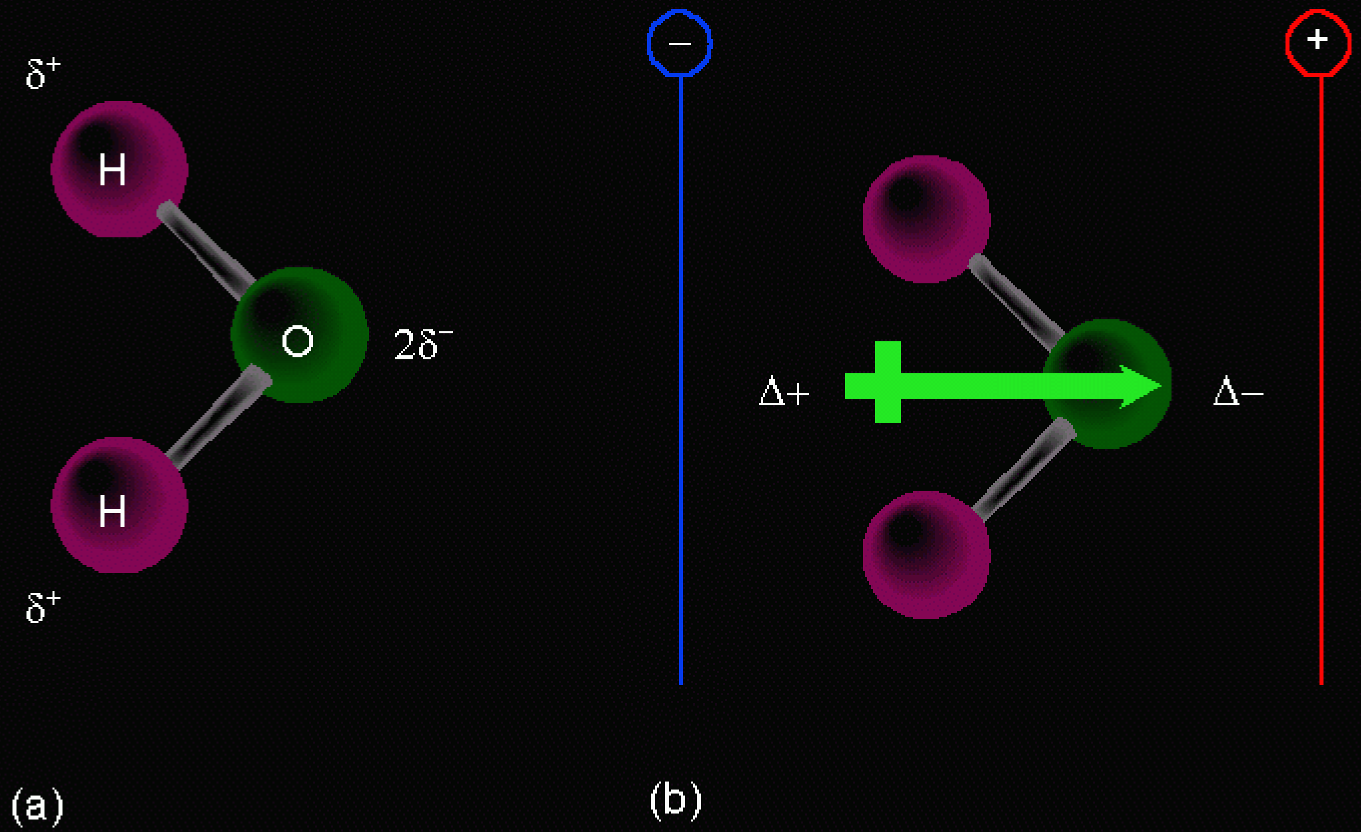


Dipole-Dipole Attractions

Attraction between oppositely charged regions of neighboring molecules.



The water dipole



Relative magnitudes of forces

The types of bonding forces vary in their strength as measured by average bond energy.

Strongest

Covalent bonds (400 kcal)

Hydrogen bonding (12-16 kcal)

Dipole-dipole interactions (2-0.5 kcal)

Weakest

London forces (less than 1 kcal)