

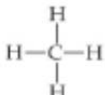
R (universal gas const.):  $8.314472 \text{ J/K} \cdot \text{mol}$   
 $1\text{m}^3 = 1000\text{l}$   
 $1 \text{ atm} = 101.325 \text{ Pa}$   
 $1 \text{ MPa} = 1 \text{ N/mm}^2 = 10 \text{ bar}$

$N_a$  (Avogadro const.):  $6.022141 \cdot 10^{23}$   
 $1 \text{ amu} = 1.66054 \cdot 10^{-24} \text{ g}$   
 $1 \text{ e}^- = 1.602 \cdot 10^{-19} \text{ C}$   
 $1 \text{ \AA} = 10^{-10} \text{ m}$

**Molecule:** Group of atoms bonded together

**Compound:** Substance made of two or more different kinds of elements

**Mixture:** Two or more Substances, where each substance can be separated

**CH<sub>4</sub>:** molecular formula  : structural formula perspective drawing, ball-stick-model, space filling model

**Atom Radius:** 1-5 Å **Nucleus Radius:** ca.  $10^{-4} \text{ \AA}$  **Nucleus Density:**  $10^{14} \text{ g/cm}^3$

$^{12}_6\text{C}$  12: mass number 6: atomic number C: elemental symbol  
mass number = protons + neutrons atomic number = protons or electrons

**1 amu** (atomic mass unit) = 1/12 weight of  $^{12}_6\text{C}$  =  $1.66054 \cdot 10^{-24} \text{ g}$  = 1 proton = 1 neutron

**Alkali metals:** 1A Li, Na, K, ...

**Alkaline earth metals:** 2A Be, Mg, Ca, ...

**Chalcogenes:** 6A O, S, Se, ...

**Halogenes:** 7A F, Cl, Br, ...

**Noble gases** (or rare gases): 8A He, Ne, Ar, ...

Combination Reactions:  $A + B \rightarrow C$  Decomposition Reactions:  $C \rightarrow A + B$

1 mole = number of atoms in 12 g of  $^{12}\text{C}$

molar mass = mass in grams/mol of a substance = atomic weight

**Ideal Gas equation:**  $PV = nRT$  P: Pressure V: Volume n: number of moles R: Gas Const. T: Temp.

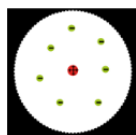
**Molar mass of a gas:**  $M = d \cdot R \cdot T / P$  M: gram/mol d: mass/volume

**Molecular speed:**  $\text{KE (kin. energ.)} = \frac{1}{2} m (u_{\text{rms}})^2$   $u_{\text{rms}} = (3 \cdot R \cdot T / M)^{1/2}$  (avg. Molecule speed)

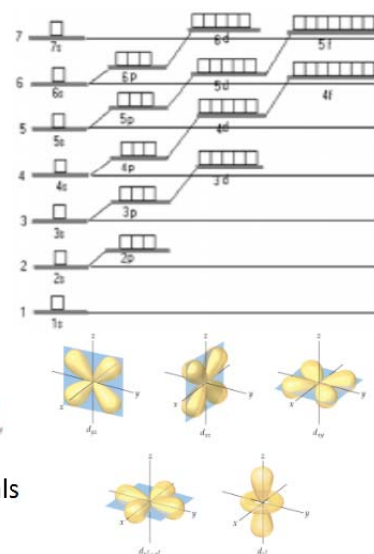
**Van der Waals eq.:**  $\left(P + \frac{n^2 a}{V^2}\right)(V - nb) = nRT$  (use when above 10 atm)



Plum Pudding model  
Thomson model



Rutherford model  
electrons orbit nucleus  
Bohr model: with orbit jumps

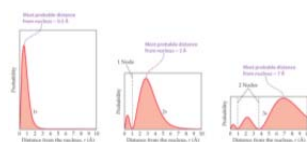


Principal quantum number (n): Shell 1, 2, 3, ...

Angular momentum quantum number (l): s, p, d, f (n-1 for a Shell n)

magnetic quantum number (m): 1 for s, 3 for p, 5 for d, 7 for f.

spin quantum number (s):  $\frac{1}{2}$  or  $-\frac{1}{2}$



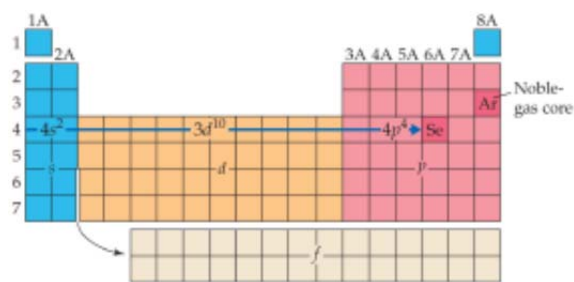
s orbitals: 1s, 2s, 3s

s orbitals  
 $2 \text{ e}^-$

p orbitals  
 $6 \text{ e}^-$

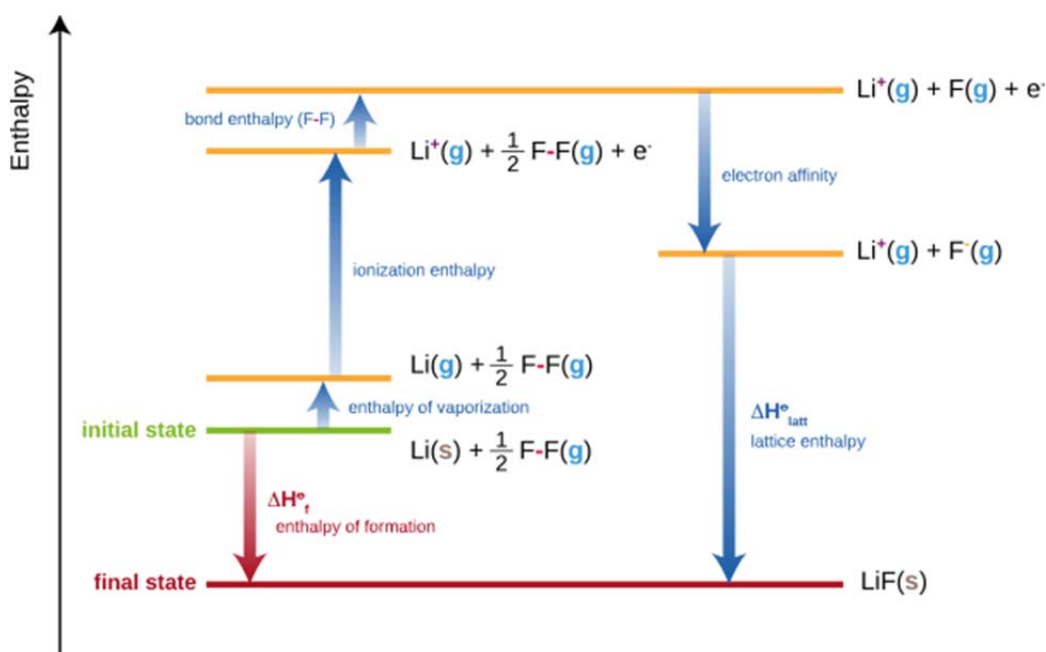
d orbitals  
 $14 \text{ e}^-$

**Effective nuclear charge:**  $Z_{\text{eff}} = Z - S$      $Z$ : nuclear charge     $S$ : screening constant = nr. core electrons (not shell)



**Ionic bond:** e.g. Salt ( $\text{Na}^+ \text{Cl}^-$ )    **covalent bond:** e.g. Water ( $\text{H}_2\text{O}$ )    **metallic bond:** e.g. Fe  
 $\Delta \text{EN}$  (electronegativity)  $> 1.7$      $\Delta \text{EN} < 1.7$

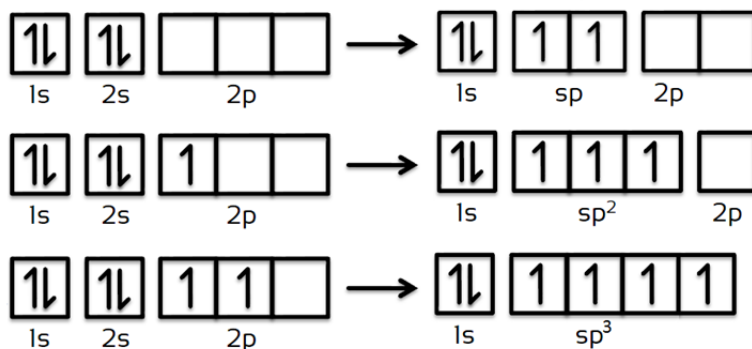
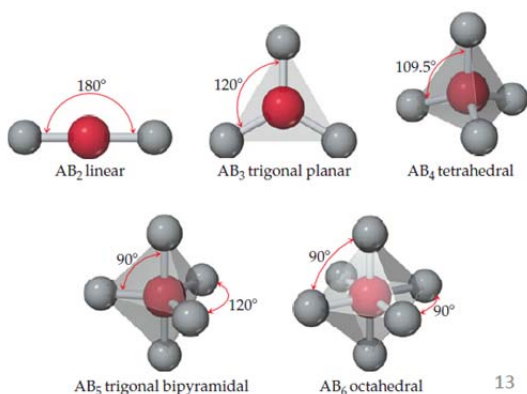
Energetics of ionic bonding:



**Force between 2 charges:**  $F = \frac{q_1 q_2}{4\pi\epsilon_0 r^2}$     **Lattice enthalpy:**  $E_c = \frac{-q_1 q_2}{4\pi\epsilon_0 r} \cdot N_A [E_c]$   
 $N_A = 6.022141 \cdot 10^{23} \text{ mol}^{-1}$     Ladung  $e^-, p^+ = 1.602 \cdot 10^{-19} \text{ C}$      $\epsilon_0 = 8.85418 \cdot 10^{-12} \text{ C}^2/(\text{Nm}^2)$

**Dipole moment  $\mu$ :**  $\mu = Q \cdot r$  (2 charges  $Q$  at distance  $r$ ) (quantifies bond polarity)

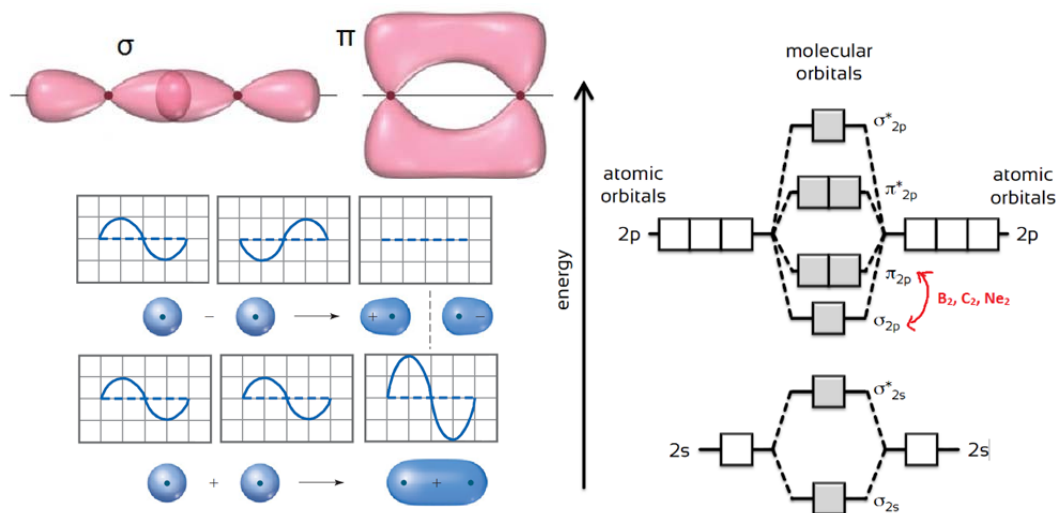
**Formal Charge:** (number of usual valence electrons) - (number of valence electrons in bond)  
 when multiple Lewis structures are possible choose the one with least formal charge.



**Single bond:** 1  $\sigma$   
**Double bond:** 1  $\sigma$  & 1  $\pi$   
**Triple bond:** 1  $\sigma$  & 2  $\pi$

Destructive addition  $\sigma^*_{1s}$   
 high energy state

Constructive addition  $\sigma_{1s}$   
 low energy state



**Bond order:**  $\frac{1}{2}$  (bonding  $e^-$  - antibonding  $e^-$ ) describes stability of bonding (use above scheme)  
 single bond  $\rightarrow$  order 1, double bond  $\rightarrow$  order 2, triple bond  $\rightarrow$  order 3

**Paramagnetic:** a Molecule has 1+ unpaired electrons (is attracted to magnetic field)

**Diamagnetic:** a Molecule has no unpaired electrons (is weakly repelled by a magnetic field)

**Open System:** heat and matter can enter/leave

**Closed System:** heat can enter/leave, but matter remains constant.

**Isolated System:** heat and matter remain const.

**1<sup>st</sup> law of thermodynamics:**  $\Delta E = q + w$   $\Delta E$ : Internal energy  $q$ : gain of heat in system  $w$ : work put into system

**Pressure-Volume work:**  $w = -P \Delta V$   $P$ : Pressure (Const.)  $\Delta V$ : Change in Volume

Isothermal expansion of gas:  $w = -nRT \ln(V_2/V_1)$

**Enthalpy:**  $H = E + PV$  when  $P$  Const.  $\rightarrow \Delta H = q_p = \Delta E + P \Delta V$

**Endothermic process:** absorbs heat from the surroundings ( $\Delta H > 0$ )

**Exothermic process:** releases heat to the surroundings ( $\Delta H < 0$ )

**Specific heat capacity:**  $C_s$  = heat capacity for 1g **Molar heat capacity:**  $C_m$  heat capacity for 1 mol  
 $q = C_s \cdot m \cdot \Delta T$   $m$ : grams of substance  $\Delta T$ : temperature change  $q$ : heat transferred

**Enthalpy of formation:**  $\Delta H^\circ_f$  Enthalpy per mol needed to form a substance (sources:  $C_{(Graphite)}$ ,  $O_2$ ,  $H_2$ )

**Spontaneity:** spontaneous behaviour is not reversible.

**Reversibility:** a reversible system is one that changes direction with an infinitesimal condition change

**Entropy:**  $\Delta S = q_{rev}/T$   $q_{rev}$ : heat transferred reversibly ( $\Delta S=0$ : reversible,  $\Delta S>0$ : irreversible,  $\Delta S<0$ : no reaction)

$\Delta S_{tot} = \Delta S_{sys} + \Delta S_{surr}$   $\Delta S_{sys} = \sum \Delta S_{products} - \sum \Delta S_{reactants}$   $\Delta S_{surr} = -\Delta H/T$

Isothermal expansion of gas:  $\Delta S = nR \ln(V_2/V_1)$

**2<sup>nd</sup> law of thermodynamics:**  $\Delta S$  is positive for irreversible, and 0 for reversible processes. Entropy increases.

**3<sup>rd</sup> law of thermodynamics:**  $\Delta S$  of a perfect crystal at 0°K is exactly equal to zero

**Gibbs free energy:**  $\Delta G = \Delta H - T \Delta S$   $\Delta G$  must be negative for a process to be spontaneous

$\Delta G = \Delta G^\circ + RT \ln(Q)$   $\Delta G^\circ$ : standard molar Gibbs energy  $Q$ : reaction quotient (=  $K_{eq}$  at equilibrium)

**Rates of Reaction:** for  $aA + bB \rightarrow cC + dD$   $rate = -\frac{1}{a} \frac{\Delta[A]}{\Delta t} = -\frac{1}{b} \frac{\Delta[B]}{\Delta t} = \frac{1}{c} \frac{\Delta[C]}{\Delta t} = \frac{1}{d} \frac{\Delta[D]}{\Delta t}$  [rate]=mol/s

**Rate laws:**  $rate = k[A]^m[B]^n$   $k$ : rate coefficient ( $\neq$  eq. const.  $K_{eq}$ )  $m, n$ : reaction orders

**Reaction order:** sum of orders of all components in the rate law (e.g.  $m+n$ )

**Rate law for elementary reactions:** Molecularity = Reaction order  $A \rightarrow \dots: k[A]$   $A+A \rightarrow \dots: k[A]^2$   $A+B \rightarrow \dots: k[A][B]$

**Molecularity:** Number of molecules that participate as reactants in an elementary reaction (uni-, bi-molecular)

|                               |                          |  |                        |
|-------------------------------|--------------------------|--|------------------------|
| <b>Zero-order reaction:</b>   | rate = k                 | $[A]_t = kt + [A]_0$                             |                        |
| <b>First order reaction:</b>  | rate = k[A]              | $[A]_t = [A]_0 \cdot e^{-kt}$                    | $t_{1/2} = \ln(2)/k$   |
| <b>Second order reaction:</b> | rate = k[A] <sup>2</sup> | $1/[A]_t = kt + 1/[A]_0$                         | $t_{1/2} = 1/(k[A]_0)$ |
|                               | rate = k[A][B]           | $\ln([B][A]_0 / ([A][B]_0)) = ([B]_0 - [A]_0)kt$ |                        |

**Q10 rule:** Temperature increase of 10°K → reaction rate increase of 2-3x

**Activation Energy  $E_a$ :** Energy needed to start reaction. "rate" is proportional to  $E_a$  (not proportional to  $\Delta E$ )

**Maxwell-Boltzmann:**  $f = e^{-E_a/RT}$  f: fraction of molecules with energy >  $E_a$

**Arrhenius equation:**  $k = Ae^{-E_a/RT}$  k: rate coefficient A: Frequency factor.

**Elementary reactions:** reactions that occur in a single step.

**Catalyst:** provides a new mechanism which has lower  $E_a$  or assists in orienting reactants to increase A.

**Equilibrium constant:**  $K_c = \frac{[C]^c[D]^d}{[A]^a[B]^b}$   $aA + bB \rightleftharpoons cC + dD$  (for concentrations)  
 concentration of solids and pure liquids (e.g. water) are constant and have no effect on K.  
 if  $K > 1$ : equilibrium favors products (right); if  $K < 1$  equilibrium favors reactants (left)  
 $K_p = \frac{P_C^c P_D^d}{P_A^a P_B^b}$   $K_p = K_c(RT)^{\Delta n}$   $\Delta n$ : mol prod. – react. of gas (for partial pressures)

**Le Chatelier's Principle:** A system will shift its equilibrium so as to counteract the disturbance (change in T, P, n)

**Acid:** proton ( $H^+$ ,  $p^+$ ) donor (e.g. HCl) **Base:** proton acceptor (e.g.  $F^-$ ) **amphiprotic:** acid and base (e.g.  $H_2O$ )

**Conjugate base:** dissociated form of an acid (acid +  $H^+$ )

**Conjugate acid:** associated form of a base (base +  $H^+$ )

**Water auto-ionisation:**  $K_w = [H_3O^+][OH^-] = 10^{-14}$  (at 25°C)

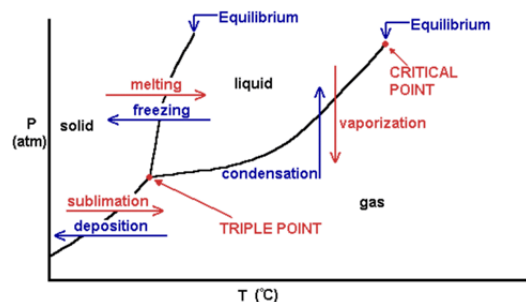
**pH** =  $-\log[H_3O^+] = -\log[H^+]$  acidic solution: pH < 7 basic solution: pH > 7

**pOH** =  $-\log[OH^-]$  pH + pOH = pK<sub>w</sub> = 14

**Dissociation constant:**  $K_a = [H_3O^+][A^-]/[HA]$   $pK_a = -\log(K_a)$   
 larger  $K_a$  → smaller  $pK_a$  → stronger acid

**Buffer equation:**  $pK_a = pH - \log([base] / [acid])$

**Phase diagram:**



**Intermolecular forces:**

dispersion forces: (weak) temporary polarization. Bigger molecule → stronger force

dipole-dipole force:  $\Delta EN$  (electronegativity) > 0.5. Greater  $\Delta EN$  → stronger force

hydrogen bonding force: (strong)  $-X \cdots H-X$  with X: N, O or F

**Solubility product:**  $K_{sp} = [A^+][B^-]$   $AB_{(s)} \rightleftharpoons A^+_{(aq)} + B^-_{(aq)}$  (Salt)

**Molarity (M):** mole/liter **Molality (m):** mole/kilogram **mole fraction ( $X_A$ ):** mole of A/total mole  
**parts per billion (ppb):** mass of A/total mass \*  $10^9$  **parts per million (ppm):** mass of A/total mass \*  $10^6$   
**mass percentage (% of A):** mass of A/total mass \* 100

**Osmosis:**  $\pi = (n/V)RT = MRT$   $\pi$ : osmotic pressure M: Molarity

**Raoult's law:**  $P_A = X_A P_A^\circ$   $P_A$ : partial vapour pressure of A  $X_A$ : % mol of A in vapour  $P_A^\circ$ : pressure if 100% A

**Depression of freezing point:**  $\Delta T_f = K_f m_i$   $\Delta T_f$ : change in freezing point  $K_f$ : cryoscopic const.  $m_i$ : mol/kg solved

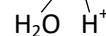
**Colloids:** very fine particles in solvents (e.g. Fog, Milk, Smoke, ...)

**Oxidation:** loss of electrons**Reduction:** gain of electrons**Oxidation number (ON):**

|                   |         |                        |             |                 |                 |
|-------------------|---------|------------------------|-------------|-----------------|-----------------|
| $O^2, N^2, \dots$ | ON = 0  | $Na^+, Ca^{2+}, \dots$ | ON = charge | 1A metals       | ON = 1          |
| 2A metals         | ON = 2  | O (except with F)      | ON = -2     | H (except salt) | ON = +1 else -1 |
| F                 | ON = -1 | Cl (except with F, O)  | ON = -1     |                 |                 |

**Balance Redox reaction:**

- 1) assign ONs      2) write half cell reactions (red & ox.)      3) balance halfcells (first non-O-H, then O, H, then  $e^-$ )  
 4) combine halfcells (balance nr. of  $e^-$ )      5) cancel anything appearing twice

**Voltaic cell:** use energy of transferring  $e^-$  in redox reaction to create electric current.**Batteries:** simple voltaic cells, made to give steady power output.**Fuel cells:** fuel and oxidant are fed continuously.**Anode:** (-) high potential, source of  $e^-$  (ox.)**Cathode:** (+) low potential, dest. of  $e^-$  (red.)**Standard cell potentials:**  $E_{cell}^0 = E_{red}^0(\text{cathode}) - E_{red}^0(\text{anode})$      $E_{cell}^0$ : standard cell voltage     $E_{red}^0$ : standard cell potential**Non-standard cell potentials:**  $E_{cell} = E_{cell}^0 - \frac{RT}{nF} \ln(Q)$      $\frac{RT}{F} \approx 0.0592$  $E_{cell}$ : cell voltage    n: nr of electrons transferred    Q: reaction quotient (K at eq.)**Gibbs energy in  $e^-$  transfer:**  $\Delta G = -nFE$     n: nr of transferred  $e^-$     F: Faraday const.    E: voltage