

# Chemistry D-MAVT

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## 1 Basics

### 1.1 Conversions, Relations and Units

mass: $[m] = kg$	mass %: $\frac{m}{m_{total}}$	kinetic energy: $E_k = \frac{1}{2}mv^2$	electron wavelength: $\lambda = \frac{h}{p_e v}$
volume: $[V] = m^3$	Avogadro's constant: $N_A = 6.022 \cdot 10^{23} \frac{1}{mol}$	potential energy: $E_p = mg\Delta h$	energy: $1eV = 1.60210^{-19} J$ $1eV = 4.18J$
molar mass: $[M] = g/mol$	mol fraction: $[x] = \frac{mol}{kg}$	electrostatic pot. energy: $E_d = \frac{1}{4\pi\epsilon_0} \frac{q_1 q_2}{d}$	pressure: $1Pa = 9.87 \cdot 10^{-6} atm$ $= 1.0 \cdot 10^{-5} bar$ $= 7.5 \cdot 10^{-3} torr$
ppm: $10^{-6}$	molality: $[M_m] = \frac{mol}{kg}$	spec. heat capacity: $c_s = \frac{q}{m\Delta T}$	STP Ideal Gas Law: $0^\circ C = 273.15K, 1bar, 1mol$
ppb: $10^{-9}$	molarity: $[M_l] = \frac{mol}{L}$	energy of photon: $E = h \cdot v = \frac{hc}{\lambda}$	STP Thermodynamics: $25^\circ C = 298.15K, 1bar, 1mol$
# particles: $[n] = mol$	length: $1 \text{ Å} = 10^{-10} m$	amount of substance: $1mol = 6.022 \cdot 10^{23}$	Planck's constant: $6.626 \cdot 10^{-34} J \cdot s$
molar mass: $[M] = \frac{kg}{mol}$	molar volume (ideal gas): $1mol = 6.022 \cdot 10^{23} \text{ atoms}$		Avogadro's number: $N_A = 6.022 \cdot 10^{23}$
molal volume (ideal gas): $V_m = 22.41L$			Volume of 1 mol: $V = N_A \cdot \Delta V$

## 1.2 Common Ions

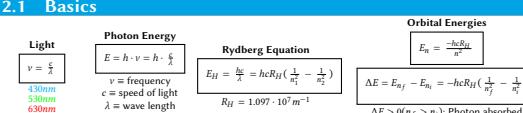
Common Anions				Common Cations			
Charge	Formula	Name	Formula	Charge	Symbol	Name	Formula
-1	H <sup>-</sup>	hydride ion	CH <sub>3</sub> COO <sup>-</sup> (or C <sub>2</sub> H <sub>5</sub> O <sub>2</sub> <sup>-</sup> )	+1	H <sup>+</sup>	hydrogen ion	NH <sub>4</sub> <sup>+</sup>
-1	F <sup>-</sup>	fluoride ion	ClO <sub>4</sub> <sup>-</sup>	+1	Li <sup>+</sup>	lithium ion	Cu <sup>+</sup>
-1	Cl <sup>-</sup>	chloride ion	CO <sub>3</sub> <sup>2-</sup>	+1	K <sup>+</sup>	potassium ion	Ca <sup>2+</sup>
-1	Br <sup>-</sup>	bromide ion	SO <sub>4</sub> <sup>2-</sup>	+1	Ag <sup>+</sup>	silver ion	Mg <sup>2+</sup>
-1	I <sup>-</sup>	iodide ion	NO <sub>3</sub> <sup>-</sup>	+2	Mg <sup>2+</sup>	magnesium ion	Al <sup>3+</sup>
-1	CN <sup>-</sup>	cyanide ion	MoO <sub>4</sub> <sup>2-</sup>	+2	Ca <sup>2+</sup>	calcium ion	Si <sup>4+</sup>
-1	OH <sup>-</sup>	hydroxide ion	CO <sub>2</sub> <sup>2-</sup>	+2	Na <sup>+</sup>	sodium ion	Fe <sup>3+</sup>
-2	O <sup>2-</sup>	oxide ion	SO <sub>3</sub> <sup>2-</sup>	+2	Li <sup>+</sup>	beryllium ion	Cr <sup>3+</sup>
-2	S <sup>2-</sup>	sulfide ion	CO <sub>3</sub> <sup>2-</sup>	+2	Be <sup>2+</sup>	boron ion	Al <sup>3+</sup>
-3	N <sup>3-</sup>	nitride ion	PO <sub>4</sub> <sup>3-</sup>	+3	Al <sup>3+</sup>	aluminum ion	Cr <sup>3+</sup>

## 1.3 Trends in Periodic Table of Elements

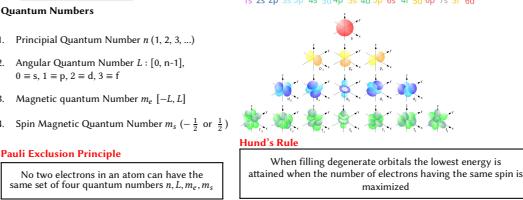
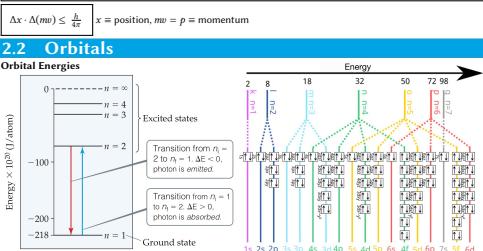
- Due to "screening", valence electrons only feel effective charge  $Z_{eff}$
- $Z_{eff}$  increases across a row
- Atomic size decreases down a column (group) and decreases across row (period)
- Ionic radii: Ions are bigger down column
- Cations are smaller than neutral atom
- Anions are larger than neutral atom
- Ionization energy: Increases across period, decreases down group

## 2 Quantum Mechanics

### 2.1 Basics



Heisenberg's Uncertainty Principle  
It is impossible to simultaneously know both the exact momentum of an electron and its exact location in space

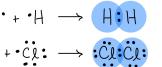


Possible Values of $n$	Possible Subshells	Possible Values of $m_l$	Number of Orbitals in Subshell	Total Number of Orbitals in Shell
1	0	1s	0	1
2	0, 1s	0, 1, -1	1, 1, 0	4
3	0, 1s, 2s	0, 1, -1, 2, -2	1, 1, 0, 1, -1	9
4	0, 1s, 2s, 3s	0, 1, -1, 2, -2, 3, -3	1, 1, 0, 1, -1, 2, -2	16

## 3 Chemical Bonds

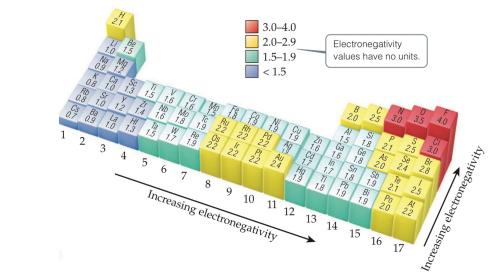
### 3.1 Covalent Bonds

- Atoms held together by sharing valence electrons
- Octet Rule: # bonds = 8 - #VE (only strictly applied for VE)
- Exceptions: Hypervalence, less than octet, odd number of VE
- for H and He: # bonds = 2 - #VE



### 3.2 Polarity and Dipole Moment

AEN < 0.5: Even distribution of VE, no dipole moment  
AEN > 0.5: Polar bond, partial negative charge at atom with higher electronegativity.



### 3.3 Lewis Structure

#### Drawing Lewis Structures

- Sum VE of all atoms
- Write symbols and connect with single bonds
- Complete octets around non-central atoms
- Place remaining VE around central atom
- Try multiple bonds if central atom does not have octet

#### Alternative Lewis Structure

- More than one Lewis Structure possible
- Calculate formal charges of each atom
- Formal charges closest to zero with negative formal charges on more EN atoms is dominant
- A molecule is most stable when it has the least overall formal charge

$$\text{Formal Charge} = \text{Atom's VE} - \frac{1}{2}(\text{Atom's bonding e's}) - (\text{Atom's non-bonding e's})$$

### 3.4 Ionic Bond

Ions held together by electrostatic attraction

Metals lose VE, non-metals gain VE

Strength quantified by lattice energy

Bond is considered ionic if AEN > 2.0

**Some Definitions:**  
Ionization Energy: Energy required to ionize (remove) e<sup>-</sup> from atom or ion  
Electron Affinity: energy change when adding and extra e<sup>-</sup> to an atom (especially exothermic)  
Lattice Energy: energy required to separate ions in ionic solid to infinite distance

#### Bookkeeping Systems

Oxidation Number: Charges atoms would have if bonds completely ionic

- Shared e<sup>-</sup> is given to more electronegative atom
- Overestimates role of electronegativity

Formal Charge: Charges atoms would have if bonding e's were shared equally

- Ignores electronegativity

Partial Charge: Somewhere in between

#### Oxidation Numbers

Rules: Atoms in elemental form: 0

Monatomic ions: **ionic charge**

Nonmetals in ionic/molecular compounds: **negative oxidation numbers**

Oxygen: -2 (except peroxide ion, O<sub>2</sub><sup>-</sup>, -1)

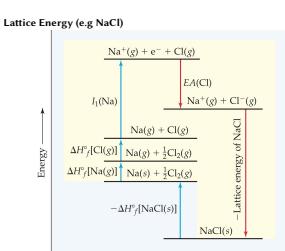
H: +1 (except if bonded to metal, -1)

F: -1 (always)

Cl, Br, I: -1 (except if bonded to oxygen)

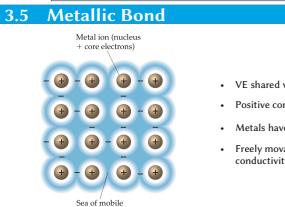
Sum of oxidation numbers for atoms in compound equals its net charge

When filling degenerate orbitals the lowest energy is attained when the number of electrons having the same spin is maximized



$$\begin{aligned} \Delta H_{lattice} &= -\Delta H_f^o[NaCl(s)] \\ &+ \Delta H_f^o[Na(g)] \\ &+ \Delta H_f^o[Cl(g)] \\ &+ I_1[Na] \\ &+ EA[Cl] \end{aligned}$$

Energy →



- Positive core surrounded by negatively charged electron cloud
- Metals have a deficit of VE and therefore do not form covalent bonds
- Freely movable electron cloud is cause for high thermal and electrical conductivity

### 3.5 Metallic Bond

Energy →

Pressure →

Temperature (°C) →

Pressure (kPa) →

Temperature (°K) →

Pressure (MPa) →

Temperature (°F) →

Pressure (Pa) →

Temperature (°R) →

Pressure (bar) →

Temperature (°C) →

Pressure (atm) →

Temperature (°F) →

Pressure (psi) →

Temperature (°R) →

Pressure (torr) →

Temperature (°K) →

Pressure (mmHg) →

Temperature (°C) →

Pressure (atm) →

Temperature (°F) →

Pressure (bar) →

Temperature (°R) →

Pressure (psi) →

Temperature (°K) →

Pressure (atm) →

Temperature (°C) →

Pressure (bar) →

Temperature (°F) →

Pressure (psi) →

Temperature (°R) →

Pressure (torr) →

Temperature (°K) →

Pressure (mmHg) →

Temperature (°C) →

Pressure (bar) →

Temperature (°F) →

Pressure (psi) →

Temperature (°R) →

Pressure (torr) →

Temperature (°K) →

Pressure (mmHg) →

Temperature (°C) →

Pressure (bar) →

Temperature (°F) →

Pressure (psi) →

Temperature (°R) →

Pressure (torr) →

Temperature (°K) →

Pressure (mmHg) →

Temperature (°C) →

Pressure (bar) →

Temperature (°F) →

Pressure (psi) →

Temperature (°R) →

Pressure (torr) →

Temperature (°K) →

Pressure (mmHg) →

Temperature (°C) →

Pressure (bar) →

Temperature (°F) →

Pressure (psi) →

Temperature (°R) →

Pressure (torr) →

Temperature (°K) →

Pressure (mmHg) →

Temperature (°C) →

Pressure (bar) →

Temperature (°F) →

Pressure (psi) →

Temperature (°R) →

Pressure (torr) →

Temperature (°K) →

Pressure (mmHg) →

Temperature (°C) →

Pressure (bar) →

Temperature (°F) →

Pressure (psi) →

Temperature (°R) →

Pressure (torr) →

Temperature (°K) →

Pressure (mmHg) →

Temperature (°C) →

Pressure (bar) →

Temperature (°F) →

Pressure (psi) →

Temperature (°R) →

Pressure (torr) →

Temperature (°K) →

Pressure (mmHg) →

Temperature (°C) →

Pressure (bar) →

Temperature (°F) →

Pressure (psi) →

Temperature (°R) →

Pressure (torr) →

Temperature (°K) →

Pressure (mmHg) →

Temperature (°C) →

Pressure (bar) →

Temperature (°F) →

## 5.4 Osmotic Pressure

The pressure required to counteract osmotic flow of a liquid is called the osmotic pressure. The osmotic flow tries to equalize concentrations across semi-permeable membranes.

$$\Pi = M \cdot RT$$

$$M = \text{molarity}$$

$$i = \text{van't Hoff factor}$$

## 5.5 Ideal Gases

Assumptions for ideal gases:

- Gas particles do not interact
- Gas particles have no volume

1<sup>st</sup> Gas (Boyle's) Law

$$P \cdot V = \text{const. if } n \& T \text{ const.}$$

2<sup>nd</sup> Gas (Charles') Law

$$\frac{V}{T} = \text{const. if } n \& P \text{ const.}$$

3<sup>rd</sup> Gas (Avogadro's) Law

$$\frac{V}{n} = \text{const. if } P \& T \text{ const.}$$

Van der Waals Equations

$$(P + \frac{a}{V^2})(V - nb) = nRT$$

a, b are correction factors

$\frac{a}{V^2}$  corrects interactions at low T.

nb corrects non-negligible volume occupied by molecules at high P

$$P_{\text{gas}} = P_{\text{atm}} + \rho gh$$

Diagram showing liquid Hg and gas pressure

$$P_{\text{gas}} = P_{\text{atm}} + \rho gh$$

At 0°C, fewer than half the molecules move at speeds greater than 500 m/s.

At 100°C, more than half the molecules move at speeds greater than 500 m/s.

$u_{\text{avg}}$  = the speed exhibited by the largest number of molecules

$u_{\text{rms}}$  = the average (mean) speed of all the molecules

$u_{\text{mp}}$  = the speed of a molecule whose kinetic energy is equal to the average (mean) kinetic energy of all the molecules

$$u_{\text{mp}} = \sqrt{\frac{2RT}{M}}$$

$$u_{\text{rms}} = \sqrt{\frac{3RT}{M}}$$

Fraction of molecules vs. Molecular speed (m/s)

Fraction of molecules vs. Molecular speed (m/s)

$$u_{\text{mp}} = \sqrt{\frac{2RT}{M}}$$

$$u_{\text{rms}} = \sqrt{\frac{3RT}{M}}$$

Standard Free Energy of Formation

$$\Delta G^\circ_f = \sum n_i \Delta G^\circ_f (\text{products}) - \sum m_i \Delta G^\circ_f (\text{reactants})$$

The Importance of T

Example

$$2O_2(g) \rightarrow 3O_2(g)$$

$$3O_2(g) \rightarrow 2O_2(g)$$

$$H_2O(l) \rightarrow H_2O(l)$$

$$H_2O(l) \rightarrow H_2O(l)$$

Temperature dependence

spontaneous at all T

nonspontaneous at all T

spontaneous at low T

spontaneous at high T

Spontaneous vs. Nonspontaneous Processes

If process is spontaneous in one direction → nonspontaneous in reverse

Nonspontaneous does not mean impossible (add energy)

Experimental conditions matter

All spontaneous processes are irreversible (requires work to return to initial state).

Reversible vs. Irreversible Process

Reversible: Process can be reversed with no change to surroundings.  $\Delta S_{\text{univ}} = 0$

Irreversible: Surroundings change when process is reversed (e.g. heat transfer)

6 Thermodynamics

## 6.1 The Three Laws of Thermodynamics

1<sup>st</sup> Law

Energy can be converted from one form to another, but it is neither created nor destroyed.

2<sup>nd</sup> Law

The entropy of the universe increases for any spontaneous process.

Reversible Process:  $\Delta S_{\text{univ}} = \Delta S_{\text{sys}} + \Delta S_{\text{surf}} = 0$

Irreversible Process:  $\Delta S_{\text{univ}} = \Delta S_{\text{sys}} + \Delta S_{\text{surf}} > 0$

3<sup>rd</sup> Law

The entropy of a pure, perfect crystalline substance at absolute zero is zero:  $S(0K) = 0$ .

There is only one possible microstate.

$$S = k \ln(V) = k \ln(1) = 0$$

6.2 System and Internal Energy

System Types and Internal Energy

Open: Matter and energy can be exchanged with surroundings

Closed: Energy can be exchanged with surroundings (but not matter)

Isolated: Neither matter nor energy is exchanged with surroundings

$$\Delta E = E_{\text{final}} - E_{\text{initial}}$$

$\Delta E > 0 \rightarrow$  system has gained E,  $\Delta E < 0 \rightarrow$  system has lost E.

Internal Energy

$$\Delta E = q + w, q = \text{heat added to system}, w = \text{work done on system}$$

$q > 0$  heat is added to system (endothermic)  $w > 0$  work done on system

$q < 0$  heat is lost by system (exothermic)  $w < 0$  work done by system

Calorimetry e.g.  $H_2O: c_p = 4.18 \frac{J}{g \cdot K}$

Heat capacity = heat required for  $\Delta T = 1K$  for specific substance

$$q = n \cdot c_m \cdot \Delta T$$

$c_m$  = molar heat capacity

$$[c_m] = \frac{J}{mol \cdot K}$$

$$q = n \cdot c_s \cdot \Delta T$$

$c_s$  = specific heat capacity

$$[c_s] = \frac{J}{kg \cdot K}$$

Exothermic Reaction

$$E_a, \text{forward} > E_a, \text{reverse}$$

$\Delta E = E_a, \text{forward} - E_a, \text{reverse}$

$$\Delta E = E_a, \text{forward} - E_a, \text{reverse}$$

Endothermic Reaction

$$E_a, \text{forward} < E_a, \text{reverse}$$

$\Delta E = E_a, \text{forward} - E_a, \text{reverse}$

$$\Delta E = E_a, \text{forward} - E_a, \text{reverse}$$

reaction coordinate

reaction coordinate