# CHEM 155 Honor General Chemistry II Equations

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### **Acid-Base Equilibria**

#### **Fundamentals**

Description	Equations
Autoionization of water	$2\mathrm{H}_2\mathrm{O} \Longrightarrow \mathrm{H}_3\mathrm{O}^+ + \mathrm{OH}^- \ K_w = [\mathrm{H}_3\mathrm{O}^+][\mathrm{OH}^-] = 10^{-14}$
pH function	$\mathrm{pH} = -\log\left[\mathrm{H_3O}^+\right]$
Acid dissociation constant	$egin{aligned} \mathbf{H}\mathbf{A} + \mathbf{H}_2\mathbf{O} & & \mathbf{H}_3\mathbf{O}^+ + \mathbf{A}^- \ K_a & = rac{[\mathbf{H}_3\mathbf{O}^+][\mathbf{A}^-]}{\mathbf{H}\mathbf{A}} \end{aligned}$
Base dissociation constant	$egin{aligned} \mathbf{B} + \mathbf{H_2O} & \Longrightarrow \mathbf{HB}^+ + \mathbf{OH}^- \ K_b &= rac{[\mathbf{HB}^+][\mathbf{OH}^-]}{[\mathbf{B}]} \end{aligned}$
Relationship between dissociation constants	$egin{aligned} K_w &= K_a K_b \ \mathrm{p} K_a + \mathrm{p} K_b &= \mathrm{p} K_w = 14 \end{aligned}$
Indicators	$egin{aligned} rac{ ext{HIn} +  ext{H}_2 ext{O}}{ ext{Eq.}} & \stackrel{ ext{H}_3 ext{O}^+}{ ext{In}^-} \ rac{ ext{[HIn]}}{ ext{[In}^-]} \end{aligned}$

#### **Buffer and titration**

Description	Equations
<b>Henderson–Hasselbalch equation</b> pH of a buffer	$\mathrm{pH} = \mathrm{p}K_a + \lograc{[\mathrm{A}^-]_0}{[\mathrm{HA}]_0}$
Titration curve at half equivalence point	$\mathrm{pH}=\mathrm{p}K_a$ (where $[\mathrm{HA}]=[\mathrm{A}^-]$ )
Titration curve until equivalence point $(0 < V < V_e)$	(1) Stoichiometric calculation of neutralization gives new acid/base concentration. (2) calculate pH using buffer (H-H equation).
Titration curve at equivalence point $V=V_e$	$egin{aligned}  ext{mol acid} &=  ext{mol base} \ c_0 V_0 &= c_e V_e \end{aligned}$
Titration curve beyond equivalence point $V>V_e$	Calculate pH using excess base that wasn't consumed in the neutralization reaction.

### Polyprotic acid

Description	Equations
Polyprotic acid reactions	$egin{aligned} \mathrm{H}_2\mathrm{A} + \mathrm{H}_2\mathrm{O} & \Longrightarrow \mathrm{HA}^- + \mathrm{H}_3\mathrm{O}^+(K_{a1}) \ \mathrm{HA}^- + \mathrm{H}_2\mathrm{O} & \Longrightarrow \mathrm{A}^{2-} + \mathrm{H}_3\mathrm{O}^+(K_{a2}) \ \mathrm{A}^{2-} + \mathrm{H}_2\mathrm{O} & \Longrightarrow \mathrm{HA}^- + \mathrm{OH}^-(K_{b1}) \ \mathrm{HA}^- + \mathrm{H}_2\mathrm{O} & \Longrightarrow \mathrm{H}_2\mathrm{A} + \mathrm{OH}^-(K_{b2}) \end{aligned}$
Relationship between dissociation constants	$K_{b1} = rac{K_w}{K_{a2}} \ K_{b2} = rac{K_w}{K_{a1}}$
Effect of pH on solution composition	$\begin{split} \frac{[\mathrm{HA}^-]}{[\mathrm{H}_2\mathrm{A}]} &= \frac{K_{a1}}{[\mathrm{H}_3\mathrm{O}^+]} \\ \frac{[\mathrm{A}^{2-}]}{[\mathrm{HA}^-]} &= \frac{K_{a2}}{[\mathrm{H}_3\mathrm{O}^+]} \\ \mathrm{p}K_{a1} \text{ and } \mathrm{p}K_{a2} \text{ are located at the} \\ \mathrm{intersections of titration curve (half equivalence point).} \end{split}$

### **Exact treatment of acid-base equilibria**

Description	Equations
pH of dilute weak acid $x \equiv [{ m H_3O}^+]$	$x^3 + (c_b + K_a)x^2 - (K_w + c_a K_a)x - \ K_a K_w = 0$
Amphotaric equilibriua $ ext{for [amph]}\gg K_{a1} \  ext{[amph]}K_{a2}\gg K_w$	$egin{aligned}  ext{pH} &pprox rac{1}{2}( ext{p}K_{a1}+ ext{p}K_{a2}) \ [ ext{H}_3 ext{O}^+] &pprox \sqrt{K_{a1}K_{a2}} \end{aligned}$

### **Solution Equilibria**

Description	Equations
Solubility product	$egin{aligned} \mathbf{M}_a\mathbf{X}_b & \Longrightarrow a\mathbf{M}^{b+} + b\mathbf{X}^{a-} \ K_{sp} &= [\mathbf{M}^{b+}]^a[\mathbf{X}^{a-}]^b \end{aligned}$
Complex ion equilibria Formation constant	$egin{aligned} &\operatorname{M}^{a+} + \operatorname{X} \Longrightarrow \operatorname{MX}^{a+}(K_1) \ &\operatorname{MX}^{a+} + \operatorname{X} \Longrightarrow \operatorname{MX}_2^{a+}(K_2) \ &\operatorname{M}^{a+} + 2\operatorname{X} \Longrightarrow \operatorname{MX}_2^{a+}(\operatorname{K}_f) \ &K_f = K_1K_2 \end{aligned}$
Selective precipitation of ions	$egin{aligned} \mathbf{M}_a \mathbf{X}_b & \Longrightarrow a  \mathbf{M}^{b+} + b  \mathbf{X}^{a-} \ [\mathbf{M}^{b+}]^a &= rac{K_{sp}}{[\mathbf{X}^{a-}]^b} \ a  \log \left[\mathbf{M}^{b+} ight] &= -b \log \left[\mathbf{X}^{a-} ight] + \log K_{sp} \end{aligned}$ The linear equation can be plotted on a log-log

Description	Equations
	M vs X graph.
Metal sulfides	$H_2S + H_2O \Longrightarrow H_3O^+ + HS^ MS + H_2O \Longrightarrow M^{2+} + HS^- + OH^-$

### **Electrochemistry**

#### **Fundamentals**

Description	Equations
Galvanic (voltaic) cells	spontaneous, produce electricity to do work
Electrolytic cells	nonspontaneous, use electricity supply to do work
cathode	reduction, gain electron
anode	oxidation, lose electron
Electrostatic potential	$E=rac{U_e}{q}$
Change in electrostatic potential energy	$\Delta U_e = q \Delta E$
Total charge passed in current in given time	Q=it
Moles of electrons transferred in current in given time	$n=rac{it}{F}$
pH meter reaction at cathode	$2\mathrm{H_3O^+} + 2\mathrm{e^-} \longrightarrow \mathrm{H_2} + 2\mathrm{H_2O}$
pH meter reaction at anode	$ m H_2 + 2H_2O \longrightarrow 2H_3O^+ + 2e^-$

### **Cell potentials and Gibbs free energy**

Description	Equations
Electrical work $(\Delta P=0;\Delta T=0)$	$egin{aligned} w = \Delta U_e = -QE_{ m cell} = -itE_{ m cell} \ w_{ m rev} = \Delta G \end{aligned}$
Standard cell potential	$E_{ m cell}^\circ = E_{ m red}^\circ({ m cathode}) - E_{ m red}^\circ({ m anode})$
Change in Gibbs free energy at standard conditions and standard cell potential	$\Delta G^{\circ} = -nFE_{ m cell}^{\circ}$
Change in Gibbs free energy at standard conditions and equilibrium constant	$\Delta G^\circ = -RT \ln K$
Cell potential at standard conditions	$E_{ ext{cell}}^{\circ} = rac{RT}{nF} \ln K = rac{0.0257  ext{V}}{n} \ln K$

#### **Description Equations**

$$\Delta G = \Delta G^\circ + RT \ln Q$$

#### **Concentration effect and Nerst Equation**

Description	Equations
Nerst Equation cell potential at nonstandard conditions	$E=E^{\circ}-rac{RT}{nF}\ln Q$
	$E=E^{\circ}-rac{0.0592  ext{V}}{n}\log Q  ext{ (at } 25^{\circ} ext{C})$
Measuring equilibrium constant from standard cell potential	$egin{aligned} \ln K &= rac{nF}{RT} E_{ ext{cell}}^{\circ}  ext{ (at 25^{\circ}C)} \ \log K &= rac{n}{0.0592  ext{V}} E_{ ext{cell}}^{\circ}  ext{ (at 25^{\circ}C)} \end{aligned}$

### **Kinetics**

#### **Rate laws**

Description	Equations
Rate of reaction	$a\mathrm{A} + b\mathrm{B} \longrightarrow c\mathrm{C} + d\mathrm{D} \ \mathrm{rate} = -rac{1}{a}rac{d[\mathrm{A}]}{dt} = -rac{1}{b}rac{d[\mathrm{B}]}{dt}$
	$\mathrm{rate} = rac{1}{c}rac{d[\mathrm{C}]}{dt} = rac{1}{d}rac{d[\mathrm{D}]}{dt}$
<b>First order rate law</b> Negative line in ln[A] vs t graph.	$egin{aligned}  ext{rate} &= -rac{1}{a}rac{d[ ext{A}]}{dt} = k[ ext{A}] \ \ln\left[ ext{A} ight]_t &= -akt + \ln\left[ ext{A} ight]_0 \ [ ext{A} ight]_t &= [ ext{A} ight]_0 e^{-akt} \end{aligned}$
<b>Second order rate law</b> Positive line in 1/[A] vs t graph.	$\mathrm{rate} = -rac{1}{a}rac{d[\mathrm{A}]}{dt} = k[\mathrm{A}]^2$
	$rac{1}{\left[ \mathbf{A} ight] _{t}}=rac{1}{\left[ \mathbf{A} ight] _{0}}+akt$
<b>Zeroth order rate law</b> Negative line in [A] vs t graph.	$egin{aligned}  ext{rate} &= -rac{1}{a}rac{d[ ext{A}]}{dt} = k \ [ ext{A}]_t &= -akt + [ ext{A}]_0 \end{aligned}$

#### Kinetics and chemical equilibrium

#### Principle of detailed balance

equilibrium rate of elementary reaction is balanced by (equal to) the rate of reverse reaction

$$egin{aligned} a\,\mathrm{A} + b\,\mathrm{B} & \stackrel{k_{I}}{\rightleftharpoons} c\,\mathrm{C} + d\,\mathrm{D} \ k_{1}[\mathrm{A}]^{a}[\mathrm{B}]^{b} &= k_{-1}[\mathrm{C}]^{c}[\mathrm{D}]^{d} \ K_{1} &= rac{[\mathrm{C}]^{c}[\mathrm{D}]^{d}}{[\mathrm{A}]^{a}[\mathrm{B}]^{b}} \ K_{1} &= rac{k_{1}}{k_{-1}} \end{aligned}$$

Overall relationship between equilibrium constant and rate constant

$$K = \prod_i K_i = rac{\prod_i k_i}{\prod_i k_{-i}}$$

#### Steady-state approximation

#### Description

#### **Equations**

#### **Steady-state approximation**

no single step in the reaction is much slower than the others; assume concentration of intermediates remain constant throughout reaction (B is neighboring molecule)

(Specific reaction may differ)

$$egin{aligned} \mathbf{A} &\longrightarrow \mathbf{C} \; ext{(overall)} \ \mathbf{A} + \mathbf{B} & \stackrel{k_I}{\longleftrightarrow} \mathbf{I} + \mathbf{B} \ \mathbf{I} & \stackrel{k_2}{\longleftrightarrow} \mathbf{C} \ & \frac{d[\mathbf{I}]}{dt} = 0 = k_1[\mathbf{A}][\mathbf{B}] - k_{-1}[\mathbf{I}][\mathbf{B}] - k_2[\mathbf{I}] \ & [I] = rac{k_1[\mathbf{A}][\mathbf{B}]}{k_{-1}[\mathbf{B}] + k_2} \ & ext{rate} = rac{d[\mathbf{C}]}{dt} = k_2[\mathbf{I}] = rac{k_1k_2[\mathbf{A}][\mathbf{B}]}{k_{-1}[\mathbf{B}] + k_2} \end{aligned}$$

$$E + S \xrightarrow{k_1} P$$
 (overall)

$$E + S \stackrel{k_1}{\rightleftharpoons} ES$$

$$\mathrm{ES} \stackrel{k_2}{\longrightarrow} \mathrm{E} + \mathrm{P}$$

$$[E_T] \ \equiv [E] + [ES] \ \Longrightarrow$$

$$[E] = [E_T] - [ES]$$

#### **Enzyme Kinetics (Michaelis-Menten)**

follows analysis from steady-state approximation: intermediate [ES] remains constant; total enzyme  $[E_T]$  remains constant

$$rac{d[\mathrm{ES}]}{dt} = 0 = k_1[\mathrm{E}][\mathrm{S}] - k_{-1}[\mathrm{ES}] - \ k_2[\mathrm{ES}]$$

$$0 = k_1 [\mathrm{E_T}] [\mathrm{S}] - k_1 [\mathrm{ES}] [\mathrm{S}] - k_{-1} [\mathrm{ES}] - k_2 [\mathrm{ES}]$$

$$[{
m ES}] = rac{k_1 [{
m E_T}] [{
m S}]}{k_1 [{
m S}] + k_{-1} + k_2} = rac{[{
m E_T}] [{
m S}]}{[{
m S}] + K_m}$$

Michaelis-Menten equation

rate of enzyme catalysis

$$ext{rate} = rac{d[ ext{P}]}{dt} = k_2[ ext{ES}] = rac{k_2[ ext{E}_{ ext{T}}][ ext{S}]}{[ ext{S}] + K_m}$$

Description	Equations
Michaelis-Menten constant	$K_m=rac{k_{-1}+k_2}{k_1}$
Maximum rate of enzyme catalysis $([\mathrm{S}]\gg K_m)$	$egin{aligned} rac{d[ ext{P}]}{dt} &= rac{k_2[ ext{E}_{ ext{T}}][ ext{S}]}{[ ext{S}] + K_m} = rac{V_{ ext{max}}[ ext{S}]}{[ ext{S}] + K_m} \ V_{ ext{max}} &= k_2[ ext{E}_{ ext{T}}] \end{aligned}$
Experimental determination of Michaelis- Menten constant	$K_m = [\mathrm{S}] \left( \left( rac{V_{\mathrm{max}}}{dP/dt}  ight) - 1  ight)$
Observation from dP/dt vs. [S] graph	When $[\mathrm{S}]=K_m$ , $\dfrac{d[\mathrm{P}]}{dt}=\dfrac{1}{2}V_{\mathrm{max}}$
	When $[\mathrm{S}]  o \infty$ , $\dfrac{d[\mathrm{P}]}{dt}  o V_{\mathrm{max}}$
Turnover number of enzyme (when saturated, $[E_{\mathrm{T}}]=[ES]$ )	$k_{ m cat} \equiv k_2 = rac{V_{ m max}}{ m [E_T]}$
Linearization of Michaelis-Menten equation	$rac{1}{dP/dt} = \left(rac{K_m}{V_{ m max}} ight)rac{1}{[{ m S}]} + rac{1}{V_{ m max}}$

### **Effect of temperature on reaction rates**

Description	Equations
<b>Arrhenius equation</b> temperature dependence of reaction rate	$k=Ae^{-E_a/RT}$
<b>Linearization of Arrhenius equation</b> experimental determination of activation energy	$egin{aligned} \ln k &= \ln A - rac{E_a}{RT} \ \ln rac{k_2}{k_1} &= -rac{E_a}{R} \left(rac{1}{T_2} - rac{1}{T_1} ight) \end{aligned}$

### **Nuclear Chemistry**

#### **Baryons and leptons**

Baryon number is conserved.

Types of Baryon	Symbol	Baryon Number	Charge
Proton	$\mathbf{p}^+$	+1	+1
Antiproton	$ar{p}$	-1	-1
Neutron	n	+1	0
Antineutron	$ar{ extbf{n}}$	-1	0

Lepton number is conserved.

Types of Lepton	Symbol	Lepton Number	Charge
Electron	$\mathrm{e}^-$ , $eta^-$	+1	-1
Positron	$\mathrm{e}^+$ , $eta^+$	-1	+1
Neutrino	$ u_e$	+1	0
Antineutrino	$ar{ u}_e$	-1	0

### **Nuclear decay process**

Decay Type	Emitted Particle	$\Delta Z$ Atomic Number	$\Delta N$ Neutron Number	$\Delta A$ Mass Number	Example
lpha decay	$_2^4\mathrm{He}$	-2	-2	-4	$^{238}\mathrm{U} \longrightarrow ^{234}\mathrm{Th} + ^{4}_{2}\mathrm{He}$
$eta^-$ decay	energetic ${ m e}^-,ar u_e$	+1	-1	0	$^{14}{ m C} \longrightarrow ^{14}{ m N} + eta^- + ar u_e$
$eta^+$ emission	energetic $\mathrm{e}^+,  u_e$	-1	+1	0	$^{22}{ m Na} \longrightarrow ^{22}{ m Ne} + eta^+ +  u_e$
Electron capture	$ u_e$	-1	+1	0	$^{207}{ m Bi} + { m e}^- \longrightarrow ^{207}{ m Pb} +  u_e$
$\gamma$ -ray emission	photon $h u$	0	0	0	$^{60}\mathrm{Ni}^* \longrightarrow ^{60}\mathrm{Ni} + \gamma$
Internal conversion	e <sup>-</sup>	0	0	0	$^{125}\mathrm{Sb}^m \longrightarrow ^{125}\mathrm{Sb} + \mathrm{e}^-$

Description	Equations
Proton-neutron conversion	$egin{aligned} {}^1_1 \mathrm{p}^+ &\longrightarrow {}^1_0 \mathrm{n} + {}^0_1 \mathrm{e}^+ +  u_e \ {}^1_0 \mathrm{n} &\longrightarrow {}^1_1 \mathrm{p}^+ + {}^0_{-1} \mathrm{e}^- + ar{ u}_e \end{aligned}$

### Mass-energy relationship

Description	Equations
Mass-energy equivalence	$E^2 = m_0^2 c^4 + p^2 c^2 \ \Delta E = c^2 \Delta m \ \ (p=0)$
Spontaneity of nuclear reactions	$\Delta E < 0 \implies \Delta m < 0$
Energy equivalent conversion	$rac{1 \mathrm{u}}{931.494 \mathrm{MeV}} = 1$

### Kinetics of radioactive decay

Description	Equations
Activity	$A=-rac{dN}{dt}=kN$
Activity and number of nuclei over time	$egin{aligned} A_t &= A_0 e^{-kt} \ N_t &= N_0 e^{-kt} \end{aligned}$
Decay constant and half life	$k=rac{\ln 2}{t_{1/2}}$

### **Introduction to Quantum Mechanics**

#### Waves and energy quantization

Description	Equations
Wavelength and frequency of electromagnetic waves	$c=\lambda  u$
Quantization of energy	$arepsilon = nh u \ n=1,2,3,$
Atomic spectra of H atom	$ u = \left(rac{1}{4} - rac{1}{n^2} ight)  imes 3.29  imes 10^{15}  ext{ s}^{-1}  onumber \ n = 3, 4, 5,$
Energy quantization of photon	$\Delta E = h  u$
Frank-Hertz experiment verifies Bohr's model	$ u = rac{\Delta E}{h} = rac{eV_{ m thr}}{h}$

#### **Bohr's model**

Description	Equations
Total mechanical energy of H atom	$E=rac{1}{2}m_ev^2-rac{Ze^2}{4\pi\epsilon_0r}$
Uniform circular motion of electron a classical description	$rac{Ze^2}{4\pi\epsilon_0 r}=m_erac{v^2}{r}$
Quantized angular momentum of electron	$egin{aligned} L &= m_e v r = n rac{h}{2\pi} \ n &= 1,2,3, \end{aligned}$

Description	Equations
Allowed radius of H atom	$r_e=rac{\epsilon_0 n^2 h^2}{\pi Z e^2 m_e}=rac{n^2}{Z}a_0$
Allowed velocity of H atom	$v_n = rac{nh}{n\pi m_e r_n} = rac{Ze^2}{2\epsilon_0 nh}$
Allowed energy of H atom	$egin{align} E_n &= -rac{Z^2 e^4 m_e}{8\epsilon_0^2 n^2 h^2} \ &= -(2.18  imes 10^{-18}  ext{J}) rac{Z^2}{n^2} \ &= -(13.60  ext{eV}) rac{Z^2}{n^2} \ \end{gathered}$
	n=1,2,3,
Emission atomic spectra of H atom	$ u = (3.29  imes 10^{15} \mathrm{s}^{-1}) Z^2 \left(rac{1}{n_f^2} - rac{1}{n_i^2} ight)  onumber \ n_i > n_f = 1, 2, 3,$
Absorption atomic spectra of H atom	$ u = (3.29  imes 10^{15} \mathrm{s}^{-1}) Z^2 \left(rac{1}{n_i^2} - rac{1}{n_f^2} ight)  onumber \ n_f > n_i = 1, 2, 3,$

### **Wave-particle duality**

Description	Equations
Planck's constant lazy physicist/chemist	$\hbar=rac{h}{2\pi}$
Conservation of energy in photoelectric effect	$h u = E_{lost} + K + \Phi$
Work function of metal	$\Phi=h u_0$
Maximum kinetic energy of photoelectrons $(E_{lost}=0)$	$E_{ m max}=K=rac{1}{2}mv_e^2=rac{p^2}{2m}=h u-\Phi$
de Broglie wavelength	$\lambda = rac{h}{p} = rac{h}{mv}$
Heisenberg uncertainty principle	$(\Delta x)(\Delta p) \geq rac{h}{4\pi} = rac{\hbar}{2}$
1D standing wave	$f(x,t) = A \sin(kt) \sin(\omega t)$
Wave traveling to the right	$f(x,t) = A \sin(\omega t - kx)$

### The Schrodinger equation

Description	Equations
Time independent Schrodinger equation	$egin{split} & -rac{h^2}{8\pi^2m}rac{d^2\psi(x)}{dx^2} + V(x)\psi(x) = E\psi(x) \ & \hat{H}\Psi = E\Psi \ & \hat{H} = -rac{h^2}{8\pi^2m}rac{d^2}{dx^2} + V(x) \end{split}$
Time dependent Schrodinger equation	$\hat{H}\Psi=i\hbarrac{\partial\Psi}{\partial t}$
Normalization of wave function	$\int_{-\infty}^{\infty} \psi^* \psi \; dx = 1$
Boundary conditions of wave functions	$\lim_{x o\pm\infty}\psi(x)=0$

#### Particle in a box

Description	Equations
Wave function of 1D particles in a box	$\psi_n(x) = \sqrt{rac{2}{L}} \sin\left(rac{n\pi x}{L} ight) n  onumber \ n = 1, 2, 3,$
Allowed energy of 1D particles in a box	$E_n = rac{n^2 h^2}{8mL^2} \ n = 1, 2, 3,$
Allowed energy of 3D particles in cubic boxes	$egin{aligned} E_{n_xn_yn_z} &= rac{h^2}{8mL^2}[n_x^2 + n_y^2 + n_z^2] \ n_x &= 1,2,3, \ n_y &= 1,2,3, \ n_z &= 1,2,3, \end{aligned}$
Wave function of 2D particles in square boxes	$egin{aligned} \Psi_{n_x n_y}(x,y) \ &= \psi_{n_x}(x) \psi_{n_y}(y) \ &= rac{2}{L} \sin\left(rac{n_x \pi x}{L} ight) \sin\left(rac{n_y \pi y}{L} ight) \end{aligned}$
Wave function of 3D particles in cubic boxes	$egin{aligned} \Psi_{n_x n_y n_z}(x,y,z) \ &= \psi_{n_x}(x) \psi_{n_y}(y) \psi_{n_z}(z) = \ &\left(rac{2}{L} ight)^{3/2} \sin\left(rac{n_x \pi x}{L} ight) \sin\left(rac{n_y \pi y}{L} ight) \sin\left(rac{n_z \pi z}{L} ight) \end{aligned}$

### **Quantum Mechanics and Atomic Structure**

The hydrogen atom

Description	<b>Equations</b>
Description	Equations

Description	Equations
Principle quantum number $n$ determines energy of the electron	$egin{aligned} E_n &= -rac{Z^2 e^4 m_e}{8\epsilon_0^2 n^2 h^2} \ &= -(2.18  imes 10^{-18}  ext{J}) rac{Z^2}{n^2} \ &= -(13.60  ext{eV}) rac{Z^2}{n^2} \ n &= 1, 2, 3, \end{aligned}$
Angular momentum quantum number $l$ determines angular momentum of electron	$L^2 = l(l+1)rac{h^2}{4\pi^2} \ l = 0, 1,, n-1$
$\begin{array}{c} \textbf{Magnetic quantum number} \ m \\ \\ \text{determines z-component of angular} \\ \\ \\ \text{momentum of electron} \end{array}$	$egin{aligned} L_z &= m rac{h}{2\pi} \ m &= -l, -l+1,, 0,, l-1, l \end{aligned}$
Spin	$m_s=-rac{1}{2},rac{1}{2}$
Wave function of electron in quantum state $\left(n,l,m ight)$ have radial part and angular part	$\psi_{nlm}(r, heta,\phi)=R_{nl}(r)Y_{lm}( heta,\phi)$
Wave function as probability density	$egin{aligned} (\psi_{nlm})^2 dV &= [R_{nl}(r)]^2 [Y_{lm}]^2 dV \ dV &= r^2 \sin  heta \; dr \; d heta \; d\phi \end{aligned}$
Radial probability density (s orbital)	$r^2[R_{nl}(r)]^2 \ dr$
Average value of distance of electron from nucleus in an orbital	$ar{r}_{nl} = rac{n^2a_0}{Z}\left\{1+rac{1}{2}\left[1-rac{l(l+1)}{n^2} ight] ight\}$

### Hartree orbital model for many-electron atoms

Description	Equations
Orbital approximation for atoms	$\psi_{ ext{atom}} = \prod_i arphi_i(r_i)$
Coulomb potential of electron moving in shell n and effective nuclear charge	$V_n^{ m eff}(r) pprox -rac{Z_{ m eff}(n)e^2}{r}$

### **Quantum Mechanics and Molecular Structure**

### Exact molecular model for ${\rm H_2}^+$

Description	Equations
Born-Oppenheimer approximation	$\psipprox\psi_{e^-}+\psi_{ m nuclei}$
light slow nuclei; heavy fast electron	$E_{ m total} = E_{e^-} + E_{ m nuclei}$

## Molecular Orbital (MO) and Linear Combination of Atomic Orbitals (LCAO) Approximation

Description	Equations
MO-LCAO approximation for bonding orbital of ${\rm H_2}^+$	$1\sigma_gpprox\sigma_{g1s}=C_g[arphi_{1s}^A+arphi_{1s}^B]$
MO-LCAO approximation for antibonding orbital of ${ m H_2}^+$	$1\sigma_u^*pprox\sigma_{u1s}^*=C_u[arphi_{1s}^A-arphi_{1s}^B]$
Bond order	${ m B.O.} = rac{1}{2} ({ m bonding} \; e^ { m antibonding} \; e^-)$

### **Spectroscopy**

#### **Electronic spectroscopy**

Description	Equations
Transmittance ( $I_0$ is incident light; $I$ is transmitted light)	$T=rac{I}{I_0}$
Absorbance	$egin{aligned} A &= \log rac{I_0}{I} \ A &= -\log T \end{aligned}$
Beer's Law absorbance depends on molar absorption coefficient, concentration, and path legth	$I = I_0 10^{-arepsilon cl} \ A = arepsilon cl$

#### Vibrational spectroscopy - harmonic oscillator model

Description	Equations
Reduced mass of system	$\mu=\frac{m_1m_2}{m_1+m_2}$
Frequency	$\omega = \sqrt{rac{k}{\mu}}$
Characteristic frequency	
Vibrational energy	$E_n=(n+rac{1}{2})\hbar\omega=(n+rac{1}{2})h u \ n=1,2,3,$