

# CHEM 155 Honors General Chemistry II

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## # Acid-Base Equilibria

### | Fundamentals

Description	Equations
Autoionization of water	$2\text{H}_2\text{O} \rightleftharpoons \text{H}_3\text{O}^+ + \text{OH}^-$ $K_w = [\text{H}_3\text{O}^+][\text{OH}^-] = 10^{-14}$
pH function	$\text{pH} = -\log [\text{H}_3\text{O}^+]$
Acid dissociation constant	$\text{HA} + \text{H}_2\text{O} \rightleftharpoons \text{H}_3\text{O}^+ + \text{A}^-$ $K_a = \frac{[\text{H}_3\text{O}^+][\text{A}^-]}{[\text{HA}]}$
Base dissociation constant	$\text{B} + \text{H}_2\text{O} \rightleftharpoons \text{HB}^+ + \text{OH}^-$ $K_b = \frac{[\text{HB}^+][\text{OH}^-]}{[\text{B}]}$
Relationship between dissociation constants	$K_w = K_a K_b$ $\text{p}K_a + \text{p}K_b = \text{p}K_w = 14$
Indicators	$\text{HIn} + \text{H}_2\text{O} \rightleftharpoons \text{H}_3\text{O}^+ + \text{In}^-$ $\frac{[\text{H}_3\text{O}^+]}{K_a} = \frac{[\text{HIn}]}{[\text{In}^-]}$

### | Buffer and titration

Description	Equations
<b>Henderson–Hasselbalch equation</b> pH of a buffer	$\text{pH} = \text{p}K_a + \log \frac{[\text{A}^-]_0}{[\text{HA}]_0}$
Titration curve at half equivalence point	$\text{pH} = \text{p}K_a$ (where $[\text{HA}] = [\text{A}^-]$ )
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 $V = V_e$	$\text{mol acid} = \text{mol base}$ $c_0 V_0 = c_e V_e$
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	$\text{H}_2\text{A} + \text{H}_2\text{O} \rightleftharpoons \text{HA}^- + \text{H}_3\text{O}^+ (K_{a1})$ $\text{HA}^- + \text{H}_2\text{O} \rightleftharpoons \text{A}^{2-} + \text{H}_3\text{O}^+ (K_{a2})$ $\text{A}^{2-} + \text{H}_2\text{O} \rightleftharpoons \text{HA}^- + \text{OH}^- (K_{b1})$ $\text{HA}^- + \text{H}_2\text{O} \rightleftharpoons \text{H}_2\text{A} + \text{OH}^- (K_{b2})$

Description	Equations
Relationship between dissociation constants	$K_{b1} = \frac{K_w}{K_{a2}}$ $K_{b2} = \frac{K_w}{K_{a1}}$
Effect of pH on solution composition	$\frac{[\text{HA}^-]}{[\text{H}_2\text{A}]} = \frac{K_{a1}}{[\text{H}_3\text{O}^+]}$ $\frac{[\text{A}^{2-}]}{[\text{HA}^-]} = \frac{K_{a2}}{[\text{H}_3\text{O}^+]}$ <p><math>\text{p}K_{a1}</math> and <math>\text{p}K_{a2}</math> are located at the intersections of titration curve (half equivalence point).</p>

## | Exact treatment of acid-base equilibria

Description	Equations
pH of dilute weak acid $x \equiv [\text{H}_3\text{O}^+]$	$x^3 + (c_b + K_a)x^2 - (K_w + c_a K_a)x - K_a K_w = 0$
Amphoteric equilibria for $[\text{amph}] \gg K_{a1}$ $[\text{amph}] K_{a2} \gg K_w$	$\text{pH} \approx \frac{1}{2}(\text{p}K_{a1} + \text{p}K_{a2})$ $[\text{H}_3\text{O}^+] \approx \sqrt{K_{a1} K_{a2}}$

## # Solution Equilibria

Description	Equations
Solubility product	$\text{M}_a\text{X}_b \rightleftharpoons a \text{M}^{b+} + b \text{X}^{a-}$ $K_{sp} = [\text{M}^{b+}]^a [\text{X}^{a-}]^b$
Complex ion equilibria Formation constant	$\text{M}^{a+} + \text{X} \rightleftharpoons \text{MX}^{a+} (K_1)$ $\text{MX}^{a+} + \text{X} \rightleftharpoons \text{MX}_2^{a+} (K_2)$ $\text{M}^{a+} + 2 \text{X} \rightleftharpoons \text{MX}_2^{a+} (K_f)$ $K_f = K_1 K_2$
Selective precipitation of ions	$\text{M}_a\text{X}_b \rightleftharpoons a \text{M}^{b+} + b \text{X}^{a-}$ $[\text{M}^{b+}]^a = \frac{K_{sp}}{[\text{X}^{a-}]^b}$ $a \log [\text{M}^{b+}] = -b \log [\text{X}^{a-}] + \log K_{sp}$ <p>The linear equation can be plotted on a log-log M vs X graph.</p>
Metal sulfides	$\text{H}_2\text{S} + \text{H}_2\text{O} \rightleftharpoons \text{H}_3\text{O}^+ + \text{HS}^-$ $\text{MS} + \text{H}_2\text{O} \rightleftharpoons \text{M}^{2+} + \text{HS}^- + \text{OH}^-$

## # 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

Description	Equations
anode	oxidation, lose electron
Electrostatic potential	$E = \frac{U_e}{q}$
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	$n = \frac{it}{F}$
pH meter reaction at cathode	$2\text{H}_3\text{O}^+ + 2\text{e}^- \longrightarrow \text{H}_2 + 2\text{H}_2\text{O}$
pH meter reaction at anode	$\text{H}_2 + 2\text{H}_2\text{O} \longrightarrow 2\text{H}_3\text{O}^+ + 2\text{e}^-$

## | Cell potentials and Gibbs free energy

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

## | Concentration effect and Nerst Equation

Description	Equations
<b>Nerst Equation</b>	$E = E^{\circ} - \frac{RT}{nF} \ln Q$
cell potential at nonstandard conditions	$E = E^{\circ} - \frac{0.0592\text{V}}{n} \log Q \text{ (at } 25^{\circ}\text{C)}$
Measuring equilibrium constant from standard cell potential	$\ln K = \frac{nF}{RT} E_{\text{cell}}^{\circ} \text{ (at } 25^{\circ}\text{C)}$ $\log K = \frac{n}{0.0592\text{V}} E_{\text{cell}}^{\circ} \text{ (at } 25^{\circ}\text{C)}$

## # Kinetics

### | Rate laws

Description	Equations
Rate of reaction	$a\text{A} + b\text{B} \longrightarrow c\text{C} + d\text{D}$ $\text{rate} = -\frac{1}{a} \frac{d[\text{A}]}{dt} = -\frac{1}{b} \frac{d[\text{B}]}{dt}$

Description	Equations
	$\text{rate} = \frac{1}{c} \frac{d[\text{C}]}{dt} = \frac{1}{d} \frac{d[\text{D}]}{dt}$
<b>First order rate law</b> Negative line in $\ln[\text{A}]$ vs $t$ graph.	$\text{rate} = -\frac{1}{a} \frac{d[\text{A}]}{dt} = k[\text{A}]$ $\ln [\text{A}]_t = -akt + \ln [\text{A}]_0$ $[\text{A}]_t = [\text{A}]_0 e^{-akt}$
<b>Second order rate law</b> Positive line in $1/[\text{A}]$ vs $t$ graph.	$\text{rate} = -\frac{1}{a} \frac{d[\text{A}]}{dt} = k[\text{A}]^2$ $\frac{1}{[\text{A}]_t} = \frac{1}{[\text{A}]_0} + akt$
<b>Zeroth order rate law</b> Negative line in $[\text{A}]$ vs $t$ graph.	$\text{rate} = -\frac{1}{a} \frac{d[\text{A}]}{dt} = k$ $[\text{A}]_t = -akt + [\text{A}]_0$

## | Kinetics and chemical equilibrium

Description	Equations
<b>Principle of detailed balance</b> equilibrium rate of elementary reaction is balanced by (equal to) the rate of reverse reaction	$a \text{A} + b \text{B} \xrightleftharpoons[k_{-1}]{k_1} c \text{C} + d \text{D}$ $k_1 [\text{A}]^a [\text{B}]^b = k_{-1} [\text{C}]^c [\text{D}]^d$ $K_1 = \frac{[\text{C}]^c [\text{D}]^d}{[\text{A}]^a [\text{B}]^b}$ <div style="border: 1px solid black; padding: 5px; width: fit-content;"> <math display="block">K_1 = \frac{k_1}{k_{-1}}</math> </div>
Overall relationship between equilibrium constant and rate constant	$K = \prod_i K_i = \frac{\prod_i k_i}{\prod_i k_{-i}}$

## | Steady-state approximation

Description	Equations
<b>Steady-state approximation</b> no single step in the reaction is much slower than the others; assume concentration of intermediates remain constant throughout reaction (B is neighboring molecule) <i>(Specific reaction may differ)</i>	$\text{A} \longrightarrow \text{C} \text{ (overall)}$ $\text{A} + \text{B} \xrightleftharpoons[k_{-1}]{k_1} \text{I} + \text{B}$ $\text{I} \xrightarrow{k_2} \text{C}$ $\frac{d[\text{I}]}{dt} = 0 = k_1 [\text{A}] [\text{B}] - k_{-1} [\text{I}] [\text{B}] - k_2 [\text{I}]$ $[\text{I}] = \frac{k_1 [\text{A}] [\text{B}]}{k_{-1} [\text{B}] + k_2}$ $\text{rate} = \frac{d[\text{C}]}{dt} = k_2 [\text{I}] = \frac{k_1 k_2 [\text{A}] [\text{B}]}{k_{-1} [\text{B}] + k_2}$
<b>Enzyme Kinetics (Michaelis-Menten)</b> follows analysis from steady-state approximation: intermediate $[\text{ES}]$ remains constant; total enzyme $[\text{E}_\text{T}]$ remains constant	$\text{E} + \text{S} \longrightarrow \text{P} \text{ (overall)}$ $\text{E} + \text{S} \xrightleftharpoons[k_{-1}]{k_1} \text{ES}$ $\text{ES} \xrightarrow{k_2} \text{E} + \text{P}$ $[\text{E}_\text{T}] \equiv [\text{E}] + [\text{ES}] \implies [\text{E}] = [\text{E}_\text{T}] - [\text{ES}]$ $\frac{d[\text{ES}]}{dt} = 0 = k_1 [\text{E}] [\text{S}] - k_{-1} [\text{ES}] - k_2 [\text{ES}]$

Description	Equations
	$0 = k_1[E_T][S] - k_1[ES][S] - k_{-1}[ES] - k_2[ES]$ $[ES] = \frac{k_1[E_T][S]}{k_1[S] + k_{-1} + k_2} = \frac{[E_T][S]}{[S] + K_m}$
<b>Michaelis-Menten equation</b> rate of enzyme catalysis	$\text{rate} = \frac{d[P]}{dt} = k_2[ES] = \frac{k_2[E_T][S]}{[S] + K_m}$
Michaelis-Menten constant	$K_m = \frac{k_{-1} + k_2}{k_1}$
Maximum rate of enzyme catalysis ( $[S] \gg K_m$ )	$\frac{d[P]}{dt} = \frac{k_2[E_T][S]}{[S] + K_m} = \frac{V_{\max}[S]}{[S] + K_m}$ $V_{\max} = k_2[E_T]$
Experimental determination of Michaelis-Menten constant	$K_m = [S] \left( \left( \frac{V_{\max}}{dP/dt} \right) - 1 \right)$
Observation from dP/dt vs. [S] graph	<p>When <math>[S] = K_m</math>, <math>\frac{d[P]}{dt} = \frac{1}{2}V_{\max}</math></p> <p>When <math>[S] \rightarrow \infty</math>, <math>\frac{d[P]}{dt} \rightarrow V_{\max}</math></p>
Turnover number of enzyme (when saturated, $[E_T] = [ES]$ )	$k_{\text{cat}} \equiv k_2 = \frac{V_{\max}}{[E_T]}$
Linearization of Michaelis-Menten equation	$\frac{1}{dP/dt} = \left( \frac{K_m}{V_{\max}} \right) \frac{1}{[S]} + \frac{1}{V_{\max}}$

## | 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	$\ln k = \ln A - \frac{E_a}{RT}$ $\ln \frac{k_2}{k_1} = -\frac{E_a}{R} \left( \frac{1}{T_2} - \frac{1}{T_1} \right)$

## # Nuclear Chemistry

### | Baryons and leptons

Baryon number is conserved.

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

Lepton number is conserved.

Types of Lepton	Symbol	Lepton Number	Charge
Electron	$e^-, \beta^-$	+1	-1
Positron	$e^+, \beta^+$	-1	+1
Neutrino	$\nu_e$	+1	0
Antineutrino	$\bar{\nu}_e$	-1	0

## | Nuclear decay process

Decay Type	Emitted Particle	$\Delta Z$ Atomic Number	$\Delta N$ Neutron Number	$\Delta A$ Mass Number	Example
$\alpha$ decay	${}^4_2\text{He}$	-2	-2	-4	${}^{238}\text{U} \longrightarrow {}^{234}\text{Th} + {}^4_2\text{He}$
$\beta^-$ decay	energetic $e^-, \bar{\nu}_e$	+1	-1	0	${}^{14}\text{C} \longrightarrow {}^{14}\text{N} + \beta^- + \bar{\nu}_e$
$\beta^+$ emission	energetic $e^+, \nu_e$	-1	+1	0	${}^{22}\text{Na} \longrightarrow {}^{22}\text{Ne} + \beta^+ + \nu_e$
Electron capture	$\nu_e$	-1	+1	0	${}^{207}\text{Bi} + e^- \longrightarrow {}^{207}\text{Pb} + \nu_e$
$\gamma$ -ray emission	photon $h\nu$	0	0	0	${}^{60}\text{Ni}^* \longrightarrow {}^{60}\text{Ni} + \gamma$
Internal conversion	$e^-$	0	0	0	${}^{125}\text{Sb}^m \longrightarrow {}^{125}\text{Sb} + e^-$

Description	Equations
Proton-neutron conversion	${}_1^1\text{p}^+ \longrightarrow {}_0^1\text{n} + {}_1^0\text{e}^+ + \nu_e$ ${}_0^1\text{n} \longrightarrow {}_1^1\text{p}^+ + {}_{-1}^0\text{e}^- + \bar{\nu}_e$

## | Mass-energy relationship

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

## | Kinetics of radioactive decay

Description	Equations
Activity	$A = -\frac{dN}{dt} = kN$
Activity and number of nuclei over time	$A_t = A_0e^{-kt}$ $N_t = N_0e^{-kt}$

Description	Equations
Decay constant and half life	$k = \frac{\ln 2}{t_{1/2}}$

## # Introduction to Quantum Mechanics

### | Waves and energy quantization

Description	Equations
Wavelength and frequency of electromagnetic waves	$c = \lambda\nu$
Quantization of energy	$\varepsilon = nh\nu$ $n = 1, 2, 3, \dots$
Atomic spectra of H atom	$\nu = \left(\frac{1}{4} - \frac{1}{n^2}\right) \times 3.29 \times 10^{15} \text{ s}^{-1}$ $n = 3, 4, 5, \dots$
Energy quantization of photon	$\Delta E = h\nu$
Frank-Hertz experiment verifies Bohr's model	$\nu = \frac{\Delta E}{h} = \frac{eV_{\text{thr}}}{h}$

### | Bohr's model

Description	Equations
Total mechanical energy of H atom	$E = \frac{1}{2}m_e v^2 - \frac{Ze^2}{4\pi\epsilon_0 r}$
Uniform circular motion of electron a classical description	$\frac{Ze^2}{4\pi\epsilon_0 r} = m_e \frac{v^2}{r}$
Quantized angular momentum of electron	$L = m_e v r = n \frac{h}{2\pi}$ $n = 1, 2, 3, \dots$
Allowed radius of H atom	$r_e = \frac{\epsilon_0 n^2 h^2}{\pi Z e^2 m_e} = \frac{n^2}{Z} a_0$
Allowed velocity of H atom	$v_n = \frac{nh}{n\pi m_e r_n} = \frac{Ze^2}{2\epsilon_0 n h}$
Allowed energy of H atom	$E_n = -\frac{Z^2 e^4 m_e}{8\epsilon_0^2 n^2 h^2}$ $= -(2.18 \times 10^{-18} \text{ J}) \frac{Z^2}{n^2}$ $= -(13.60 \text{ eV}) \frac{Z^2}{n^2}$ $n = 1, 2, 3, \dots$
Emission atomic spectra of H atom	$\nu = (3.29 \times 10^{15} \text{ s}^{-1}) Z^2 \left( \frac{1}{n_f^2} - \frac{1}{n_i^2} \right)$ $n_i > n_f = 1, 2, 3, \dots$
Absorption atomic spectra of H atom	$\nu = (3.29 \times 10^{15} \text{ s}^{-1}) Z^2 \left( \frac{1}{n_i^2} - \frac{1}{n_f^2} \right)$ $n_f > n_i = 1, 2, 3, \dots$

## | Wave-particle duality

Description	Equations
Planck's constant lazy physicist/chemist	$\hbar = \frac{h}{2\pi}$
Conservation of energy in photoelectric effect	$h\nu = E_{lost} + K + \Phi$
Work function of metal	$\Phi = h\nu_0$
Maximum kinetic energy of photoelectrons ( $E_{lost} = 0$ )	$E_{\max} = K = \frac{1}{2}mv_e^2 = \frac{p^2}{2m} = h\nu - \Phi$
de Broglie wavelength	$\lambda = \frac{h}{p} = \frac{h}{mv}$
Heisenberg uncertainty principle	$(\Delta x)(\Delta p) \geq \frac{h}{4\pi} = \frac{\hbar}{2}$
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	$-\frac{\hbar^2}{2m} \frac{d^2\psi(x)}{dx^2} + V(x)\psi(x) = E\psi(x)$ $\hat{H}\Psi = E\Psi$ $\hat{H} = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V(x)$
Time dependent Schrodinger equation	$\hat{H}\Psi = i\hbar \frac{\partial \Psi}{\partial t}$
Normalization of wave function	$\int_{-\infty}^{\infty} \psi^* \psi \, dx = 1$
Boundary conditions of wave functions	$\lim_{x \rightarrow \pm\infty} \psi(x) = 0$

## | Particle in a box

Description	Equations
Wave function of 1D particles in a box	$\psi_n(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right)$ $n = 1, 2, 3, \dots$
Allowed energy of 1D particles in a box	$E_n = \frac{n^2 \hbar^2}{8mL^2}$ $n = 1, 2, 3, \dots$
Allowed energy of 3D particles in cubic boxes	$E_{n_x n_y n_z} = \frac{\hbar^2}{8mL^2} [n_x^2 + n_y^2 + n_z^2]$ $n_x = 1, 2, 3, \dots$ $n_y = 1, 2, 3, \dots$ $n_z = 1, 2, 3, \dots$



Description	Equations
Wave function of 2D particles in square boxes	$\Psi_{n_x n_y}(x, y)$ $= \psi_{n_x}(x) \psi_{n_y}(y)$ $= \frac{2}{L} \sin\left(\frac{n_x \pi x}{L}\right) \sin\left(\frac{n_y \pi y}{L}\right)$
Wave function of 3D particles in cubic boxes	$\Psi_{n_x n_y n_z}(x, y, z)$ $= \psi_{n_x}(x) \psi_{n_y}(y) \psi_{n_z}(z)$ $= \left(\frac{2}{L}\right)^{3/2} \sin\left(\frac{n_x \pi x}{L}\right) \sin\left(\frac{n_y \pi y}{L}\right) \sin\left(\frac{n_z \pi z}{L}\right)$

## # Quantum Mechanics and Atomic Structure

### | The hydrogen atom

Description	Equations
<b>Principle quantum number <math>n</math></b> determines energy of the electron	$E_n = -\frac{Z^2 e^4 m_e}{8 \epsilon_0^2 n^2 \hbar^2}$ $= -(2.18 \times 10^{-18} \text{J}) \frac{Z^2}{n^2}$ $= -(13.60 \text{eV}) \frac{Z^2}{n^2}$ $n = 1, 2, 3, \dots$
<b>Angular momentum quantum number <math>l</math></b> determines angular momentum of electron	$L^2 = l(l+1) \frac{\hbar^2}{4\pi^2}$ $l = 0, 1, \dots, n-1$
<b>Magnetic quantum number <math>m</math></b> determines z-component of angular momentum of electron	$L_z = m \frac{\hbar}{2\pi}$ $m = -l, -l+1, \dots, 0, \dots, l-1, l$
Spin	$m_s = -\frac{1}{2}, \frac{1}{2}$
Wave function of electron in quantum state $(n, l, m)$ have radial part and angular part	$\psi_{nlm}(r, \theta, \phi) = R_{nl}(r) Y_{lm}(\theta, \phi)$
Wave function as probability density	$(\psi_{nlm})^2 dV = [R_{nl}(r)]^2 [Y_{lm}]^2 dV$ $dV = r^2 \sin \theta \, dr \, d\theta \, d\phi$
Radial probability density (s orbital)	$r^2 [R_{nl}(r)]^2 \, dr$
Average value of distance of electron from nucleus in an orbital	$\bar{r}_{nl} = \frac{n^2 a_0}{Z} \left[ 1 + \frac{1}{2} \left[ 1 - \frac{l(l+1)}{n^2} \right] \right]$

### | Hartree orbital model for many-electron atoms

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

## # Quantum Mechanics and Molecular Structure

| Exact molecular model for  $\text{H}_2^+$

Description	Equations
<b>Born-Oppenheimer approximation</b> light slow nuclei; heavy fast electron	$\psi \approx \psi_{e^-} + \psi_{\text{nuclei}}$ $E_{\text{total}} = E_{e^-} + E_{\text{nuclei}}$

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

Description	Equations
MO-LCAO approximation for bonding orbital of $\text{H}_2^+$	$1\sigma_g \approx \sigma_{g1s} = C_g[\varphi_{1s}^A + \varphi_{1s}^B]$
MO-LCAO approximation for antibonding orbital of $\text{H}_2^+$	$1\sigma_u^* \approx \sigma_{u1s}^* = C_u[\varphi_{1s}^A - \varphi_{1s}^B]$
Bond order	$\text{B.O.} = \frac{1}{2}(\text{bonding } e^- - \text{antibonding } e^-)$

# Spectroscopy

| Electronic spectroscopy

Ultraviolet-Visible (UV-Vis) Spectroscopy

Description	Equations
Transmittance ( $I_0$ is incident light; $I$ is transmitted light)	$T = \frac{I}{I_0}$
Absorbance	$A = \log \frac{I_0}{I}$ $A = -\log T$
<b>Beer's Law</b> absorbance depends on molar absorption coefficient, concentration, and path length	$I = I_0 10^{-\epsilon cl}$ $A = \epsilon cl$

| Vibrational spectroscopy - harmonic oscillator model

Infrared (IR) Spectroscopy

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