CHEM 155 Honor General Chemistry II Equations

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Table of Contents

Acid-Base Equilibria

Fundamentals

Description	Equations
Autoionization of water	$2\,\mathrm{H_2O} \rightleftharpoons \mathrm{H_3O^+} + \mathrm{OH^-}$ $K_w = [\mathrm{H_3O^+}][\mathrm{OH^-}] = 10^{-14}$
pH function	$\mathrm{pH} = -\log[\mathrm{H_3O^+}]$
Acid dissociation constant	$\mathrm{HA} + \mathrm{H_2O} \rightleftharpoons \mathrm{H_3O^+} + \mathrm{A^-}$ $K_a = \dfrac{[\mathrm{H_3O^+}][\mathrm{A^-}]}{\mathrm{HA}}$
Base dissociation constant	$\mathrm{B} + \mathrm{H_2O} \rightleftharpoons \mathrm{HB^+} + \mathrm{OH^-}$ $K_b = \dfrac{[\mathrm{HB^+}][\mathrm{OH^-}]}{[\mathrm{B}]}$
Relationship between dissociation constants	$K_w = K_a K_b$ $\mathrm{p}K_a + \mathrm{p}K_b = \mathrm{p}K_w = 14$
Indicators	$\mathrm{HIn} + \mathrm{H_2O} \rightleftharpoons \mathrm{H_3O^+} + \mathrm{In^-}$ $\dfrac{[\mathrm{H_3O^+}]}{K_a} = \dfrac{[\mathrm{HIn}]}{[\mathrm{In^-}]}$

Buffer and titration

Description	Equations
Henderson–Hasselbalch equation pH of a buffer	$\mathrm{pH} = \mathrm{p}K_a + \log\dfrac{[\mathrm{A^-}]_0}{[\mathrm{HA}]_0}$
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 $V = V_e$	$\mathrm{mol\ acid} = \mathrm{mol\ base}$ $c_0 V_0 = c_e V_e$
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	$H_2A + H_2O \rightleftharpoons HA^- + H_3O^+ (K_{a1})$ $HA^- + H_2O \rightleftharpoons A^{2-} + H_3O^+ (K_{a2})$ $A^{2-} + H_2O \rightleftharpoons HA^- + OH^- (K_{b1})$ $HA^- + H_2O \rightleftharpoons H_2A + OH^- (K_{b2})$
Relationship between dissociation constants	$K_{b1} = \dfrac{K_w}{K_{a2}}$ $K_{b2} = \dfrac{K_w}{K_{a1}}$
Effect of pH on solution composition	$\dfrac{[HA^-]}{[H_2A]} = \dfrac{K_{a1}}{[H_3O^+]}$ $\dfrac{[A^{2-}]}{[HA^-]} = \dfrac{K_{a2}}{[H_3O^+]}$ pK_{a1} and pK_{a2} are located at the intersections of titration curve (half equivalence point).

Exact treatment of acid-base equilibria

Description	Equations
pH of dilute weak acid $x \equiv [H_3O^+]$	$x^3 + (c_b + K_a)x^2 - (K_w + c_aK_a)x - K_aK_w = 0$
Amphotaric equilibriua for $[amph] \gg K_{a1}$ $[amph]K_{a2} \gg K_w$	$pH \approx \dfrac{1}{2}(pK_{a1} + pK_{a2})$ $[H_3O^+] \approx \sqrt{K_{a1}K_{a2}}$

Solution Equilibria

Description	Equations
Solubility product	$M_aX_b \rightleftharpoons a\,M^{b+} + b\,X^{a-}$ $K_{sp} = [M^{b+}]^a[X^{a-}]^b$
Complex ion equilibria Formation constant	$M^{a+} + X \rightleftharpoons MX^{a+} (K_1)$ $MX^{a+} + X \rightleftharpoons MX_2{}^{a+} (K_2)$ $M^{a+} + 2\,X \rightleftharpoons MX_2{}^{a+} (K_f)$ $K_f = K_1K_2$
Selective precipitation of ions	$M_aX_b \rightleftharpoons a\,M^{b+} + b\,X^{a-}$ $[M^{b+}]^a = \dfrac{K_{sp}}{[X^{a-}]^b}$ $a\log[M^{b+}] = -b\log[X^{a-}] + \log K_{sp}$ The linear equation can be plotted on a log-log

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

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	$E = \dfrac{U_e}{q}$
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	$n = \dfrac{it}{F}$
pH meter reaction at cathode	$2\,H_3O^+ + 2\,e^- \longrightarrow H_2 + 2\,H_2O$
pH meter reaction at anode	$H_2 + 2\,H_2O \longrightarrow 2\,H_3O^+ + 2\,e^-$

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	$E^{\circ}_{\text{cell}} = E^{\circ}_{\text{red}}(\text{cathode}) - E^{\circ}_{\text{red}}(\text{anode})$
Change in Gibbs free energy at standard conditions and standard cell potential	$\Delta G^{\circ} = -nFE^{\circ}_{\text{cell}}$
Change in Gibbs free energy at standard conditions and equilibrium constant	$\Delta G^{\circ} = -RT\ln K$
Cell potential at standard conditions	$E^{\circ}_{\text{cell}} = \dfrac{RT}{nF}\ln K = \dfrac{0.0257\text{V}}{n}\ln K$

Description	Equations
Change in Gibbs free energy at nonstandard conditions	$\Delta G = \Delta G^\circ + RT \ln Q$

Concentration effect and Nerst Equation

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

Kinetics

Rate laws

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

Kinetics and chemical equilibrium

Description	Equations

Description	Equations
Principle of detailed balance equilibrium rate of elementary reaction is balanced by (equal to) the rate of reverse reaction	$a\,\mathrm{A} + b\,\mathrm{B} \underset{k_{-1}}{\overset{k_1}{\rightleftharpoons}} c\,\mathrm{C} + d\,\mathrm{D}$ $k_1[\mathrm{A}]^a[\mathrm{B}]^b = k_{-1}[\mathrm{C}]^c[\mathrm{D}]^d$ $K_1 = \dfrac{[\mathrm{C}]^c[\mathrm{D}]^d}{[\mathrm{A}]^a[\mathrm{B}]^b}$ $\boxed{K_1 = \dfrac{k_1}{k_{-1}}}$
Overall relationship between equilibrium constant and rate constant	$K = \prod\limits_i K_i = \dfrac{\prod\limits_i k_i}{\prod\limits_i k_{-i}}$

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*)	$\mathrm{A} \longrightarrow \mathrm{C}\ (\text{overall})$ $\mathrm{A} + \mathrm{B} \underset{k_{-1}}{\overset{k_1}{\longleftrightarrow}} \mathrm{I} + \mathrm{B}$ $\mathrm{I} \xrightarrow{k_2} \mathrm{C}$ $\dfrac{d[\mathrm{I}]}{dt} = 0 = k_1[\mathrm{A}][\mathrm{B}] - k_{-1}[\mathrm{I}][\mathrm{B}] - k_2[\mathrm{I}]$ $[I] = \dfrac{k_1[\mathrm{A}][\mathrm{B}]}{k_{-1}[\mathrm{B}] + k_2}$ $\text{rate} = \dfrac{d[\mathrm{C}]}{dt} = k_2[\mathrm{I}] = \dfrac{k_1 k_2[\mathrm{A}][\mathrm{B}]}{k_{-1}[\mathrm{B}] + k_2}$
Enzyme Kinetics (Michaelis-Menten) follows analysis from steady-state approximation: intermediate $[\mathrm{ES}]$ remains constant; total enzyme $[\mathrm{E_T}]$ remains constant	$\mathrm{E} + \mathrm{S} \longrightarrow \mathrm{P}\ (\text{overall})$ $\mathrm{E} + \mathrm{S} \underset{k_{-1}}{\overset{k_1}{\rightleftharpoons}} \mathrm{ES}$ $\mathrm{ES} \xrightarrow{k_2} \mathrm{E} + \mathrm{P}$ $[\mathrm{E_T}] \equiv [\mathrm{E}] + [\mathrm{ES}] \implies$ $[\mathrm{E}] = [\mathrm{E_T}] - [\mathrm{ES}]$ $\dfrac{d[\mathrm{ES}]}{dt} = 0 = k_1[\mathrm{E}][\mathrm{S}] - k_{-1}[\mathrm{ES}] - k_2[\mathrm{ES}]$ $0 = k_1[\mathrm{E_T}][\mathrm{S}] - k_1[\mathrm{ES}][\mathrm{S}] - k_{-1}[\mathrm{ES}] - k_2[\mathrm{ES}]$ $[\mathrm{ES}] = \dfrac{k_1[\mathrm{E_T}][\mathrm{S}]}{k_1[\mathrm{S}] + k_{-1} + k_2} = \dfrac{[\mathrm{E_T}][\mathrm{S}]}{[\mathrm{S}] + K_m}$
Michaelis-Menten equation rate of enzyme catalysis	$\text{rate} = \dfrac{d[\mathrm{P}]}{dt} = k_2[\mathrm{ES}] = \dfrac{k_2[\mathrm{E_T}][\mathrm{S}]}{[\mathrm{S}] + K_m}$

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

Effect of temperature on reaction rates

Description	Equations
Arrhenius equation temperature dependence of reaction rate	$k = Ae^{-E_a/RT}$
Linearization of Arrhenius equation experimental determination of activation energy	$\ln k = \ln A - \dfrac{E_a}{RT}$ $\ln \dfrac{k_2}{k_1} = -\dfrac{E_a}{R} \left(\dfrac{1}{T_2} - \dfrac{1}{T_1} \right)$

Nuclear Chemistry

Baryons and leptons

Baryon number is conserved.

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

Lepton number is conserved.

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

Nuclear decay process

Decay Type	Emitted Particle	ΔZ Atomic Number	ΔN Neutron Number	ΔA Mass Number	Example
α decay	${}^{4}_{2}\text{He}$	-2	-2	-4	${}^{238}\text{U} \longrightarrow {}^{234}\text{Th} + {}^{4}_{2}\text{He}$
β^- decay	energetic $e^-, \bar{\nu}_e$	+1	-1	0	${}^{14}\text{C} \longrightarrow {}^{14}\text{N} + \beta^- + \bar{\nu}_e$
β^+ emission	energetic e^+, ν_e	-1	+1	0	${}^{22}\text{Na} \longrightarrow {}^{22}\text{Ne} + \beta^+ + \nu_e$
Electron capture	ν_e	-1	+1	0	${}^{207}\text{Bi} + e^- \longrightarrow {}^{207}\text{Pb} + \nu_e$
γ-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	${}^{1}_{1}\text{p}^+ \longrightarrow {}^{1}_{0}\text{n} + {}^{0}_{1}\text{e}^+ + \nu_e$ ${}^{1}_{0}\text{n} \longrightarrow {}^{1}_{1}\text{p}^+ + {}^{0}_{-1}\text{e}^- + \bar{\nu}_e$

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	$\dfrac{1\text{u}}{931.494\text{MeV}} = 1$

Kinetics of radioactive decay

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

Introduction to Quantum Mechanics

Waves and energy quantization

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

Bohr's model

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

Description	Equations
Allowed radius of H atom	$r_e = \dfrac{\epsilon_0 n^2 h^2}{\pi Z e^2 m_e} = \dfrac{n^2}{Z} a_0$
Allowed velocity of H atom	$v_n = \dfrac{nh}{n\pi m_e r_n} = \dfrac{Ze^2}{2\epsilon_0 nh}$
Allowed energy of H atom	$E_n = -\dfrac{Z^2 e^4 m_e}{8\epsilon_0^2 n^2 h^2}$ $= -(2.18 \times 10^{-18}\,\text{J})\dfrac{Z^2}{n^2}$ $= -(13.60\,\text{eV})\dfrac{Z^2}{n^2}$ $n = 1, 2, 3, ...$
Emission atomic spectra of H atom	$\nu = (3.29 \times 10^{15}\text{s}^{-1})Z^2\left(\dfrac{1}{n_f^2} - \dfrac{1}{n_i^2}\right)$ $n_i > n_f = 1, 2, 3, ...$
Absorption atomic spectra of H atom	$\nu = (3.29 \times 10^{15}\text{s}^{-1})Z^2\left(\dfrac{1}{n_i^2} - \dfrac{1}{n_f^2}\right)$ $n_f > n_i = 1, 2, 3, ...$

Wave-particle duality

Description	Equations
Planck's constant lazy physicist/chemist	$\hbar = \dfrac{h}{2\pi}$
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 $(E_{lost} = 0)$	$E_{\max} = K = \dfrac{1}{2}mv_e^2 = \dfrac{p^2}{2m} = h\nu - \Phi$
de Broglie wavelength	$\lambda = \dfrac{h}{p} = \dfrac{h}{mv}$
Heisenberg uncertainty principle	$(\Delta x)(\Delta p) \geq \dfrac{h}{4\pi} = \dfrac{\hbar}{2}$
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

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

Particle in a box

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

Quantum Mechanics and Atomic Structure

The hydrogen atom

Description	Equations

Description	Equations
Principle quantum number n determines energy of the electron	$$E_n = -\frac{Z^2 e^4 m_e}{8\epsilon_0^2 n^2 h^2}$$ $$= -(2.18 \times 10^{-18}\,\text{J})\frac{Z^2}{n^2}$$ $$= -(13.60\,\text{eV})\frac{Z^2}{n^2}$$ $$n = 1, 2, 3, \ldots$$
Angular momentum quantum number l determines angular momentum of electron	$$L^2 = l(l+1)\frac{h^2}{4\pi^2}$$ $$l = 0, 1, \ldots, n-1$$
Magnetic quantum number m determines z-component of angular momentum of electron	$$L_z = m\frac{h}{2\pi}$$ $$m = -l, -l+1, \ldots, 0, \ldots, l-1, l$$
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
Born-Oppenheimer approximation 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 H_2^+	$1\sigma_g \approx \sigma_{g1s} = C_g[\varphi_{1s}^A + \varphi_{1s}^B]$
MO-LCAO approximation for antibonding orbital of 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

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

Vibrational spectroscopy - harmonic oscillator model

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