Common Equations Used in Chemistry

John Terhorst, Ph.D.

Updated February 14, 2021

Contents

1	Basic Conversions and Definitions	3				
2	Solutions	3				
3	Gases	4				
4	Thermodynamics 4.1 Heat Exchange	5 5 5 5 6 6 7				
5	Electromagnetism	8				
6	Quantum Mechanics					
7	Stoichiometry	9				
8	Electrochemistry	10				
9	Reaction Kinetics 9.1 Kinetics Data	10 11				
10	P Equilibrium 10.1 Equilibrium of Acids and Bases	14 14 14				
11	Similarity of Equations 11.1 Linear Equations with Different Temperatures	15 15 15				
12	2 Statistics	16				
13	3 Other	16				
14	l Acidities	17				

15 Compound Units

1. Basic Conversions and Definitions

Converting °F to °C:

$$^{\circ}$$
C = $(^{\circ}$ F $-$ 32 $) \times \frac{5}{9}$

Converting °C to °F:

$$^{\circ}$$
F = $\left(^{\circ}$ C $\times \frac{9}{5}\right) + 32$

Converting °C to K:

$$K = {}^{\circ}\text{C} + 273.15$$

2. Solutions

Density:

$$d = \frac{m}{V}$$

Molarity:

$$C = \frac{\text{moles of solute}}{\text{liters of solution}}$$

Molality:

$$b = \frac{\text{moles of solute}}{\text{kg of solvent}}$$

Boiling point elevation¹:

$$\Delta T_{\rm b} = i K_{\rm b} b$$

Freezing point depression:

$$\Delta T_{
m f} = i K_{
m f} b$$

Table 1: Boiling point elevation and freezing point depression constants for different solvents.

Solvent	Normal Boiling (°C)	K_{b} (°C/m)	Normal Freezing (°C)	K_{f} (°C/m)
Water	100.0	0.512	0.0	1.86
Acetic acid	118.1	3.04	16.6	3.90
Benzene	80.1	2.53	5.5	5.12
${ m Chloroform}$	61.3	3.63	-63.5	4.86
Carbon tetrachloride	76.8	5.26	-22.62	31.4
Carbon disulfide	46.2	2.42	-112.1	3.74
Nitrobenzene	210.9	5.24	5.67	6.87
D-Camphor	207.4	4.91	178.8	37.8

Osmotic pressure:

$$\pi = i \mathbf{M} R T$$

Dilution:

$$C_1V_1 = C_2V_2$$

The van't Hoff factor, i, describes the number of particles formed upon solvation. For example, for solvation of sodium chloride, $\operatorname{NaCl}(s) \longrightarrow \operatorname{Na}^+(aq) + \operatorname{Cl}^-(aq)$, i=2. For a nonelectrolyte (like glucose or benzene), i=1. This factor can deviate from ideality for highly charged ions, where ion-pairing occurs (incomplete dissociation), as is seen with CaCl_2 , where i=2.6 instead of 3.0 ($\operatorname{CaCl}_2(s) \longrightarrow \operatorname{Ca}^{2+}(aq) + 2\operatorname{Cl}^-(aq)$).

3. Gases

Ideal Gas Law, $R=0.08206~\frac{\text{L} \cdot \text{atm}}{\text{K} \cdot \text{mol}}$

$$PV = nRT$$

Boyle's Law (n, T constant):

$$P_1V_1 = P_2V_2$$

Charles' Law (n, P constant):

$$\frac{V_1}{V_2} = \frac{T_1}{T_2}$$

Avogadro's Law (P, T constant):

$$\frac{V_1}{V_2} = \frac{n_1}{n_2}$$

Gay-Lussac's Law (P, T constant):

$$\frac{P_1}{P_2} = \frac{T_1}{T_2}$$

Combined Gas Law (n is constant):

$$\frac{P_1 V_1}{T_1} = \frac{P_2 V_2}{T_2}$$

Relation of density to molar mass:

$$M = \frac{dRT}{P}$$

Dalton's Law of Partial Pressures, where $\chi_i = \text{mole fraction of species } i$ and P_T is total pressure:

$$P_i = \chi_i P_{\rm T}$$

Raoult's Law, where P_i^\star is the vapor pressure of pure substance i:

$$P_{\text{Tot}} = \chi_{\text{A}} P_{\text{A}}^{\star} + \chi_{\text{B}} P_{\text{Bb}}^{\star} + \dots$$

For ionic solutes we include the van't Hoff factor i:

$$P_i = i\chi_i P_i^{\star}$$

Root-mean-square (RMS) speed of a gas particle:

$$\mu = \sqrt{\frac{3RT}{M}}$$

Rates of Effusion by Molar Mass

$$\frac{\mathrm{rate_1}}{\mathrm{rate_2}} = \sqrt{\frac{M_2}{M_1}}$$

van der Waals equation for pressure of a non-ideal gas, where a corrects for the attractive forces between gas particles, and b corrects for the volume occupied by gas particles:

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

$$P = \frac{an^2(V - nb) - RTV^2}{V^2(nb - V)}$$

4. Thermodynamics

4.1. Heat Exchange

Heat exchange, where C_s is specific heat capacity:

$$q = mC_s\Delta T$$

Calorimetry in an imperfect calorimeter:

$$q_{\rm rxn} = mC_s\Delta T + C_{\rm cal}\Delta T$$

Heat exchange, where C_V is molar heat capacity at constant volume:

$$q = nC_V \Delta T$$

Heat exchange, where C_P is molar heat capacity at constant pressure:

$$q = nC_P \Delta T$$

4.2. Conditions

4.2.1. Definitions

• Isothermal: $\Delta T = 0$, $\Delta E = 0$, q = -w

• Adiabatic: q = 0, $\Delta E = w$

• Isobaric: $\Delta P = 0$ (constant pressure)

4.2.2. In General

• $q = nC\Delta T$

• $w = -P\Delta V$ where L·atm = 101.325 J

• $\Delta E = q + w$

• $\Delta H = \Delta E + P\Delta V + V\Delta P$

• $C_{\rm P} = \frac{5}{2}R$ and $C_{\rm V} = \frac{3}{2}R$

Table 2: Summary of thermodynamic quantities under different conditions.

Quantity	Constant P	Constant V	Adiabatic	Isothermal
Heat, q	$nC_{ m P}\Delta T$	$nC_{ m V}\Delta T$	0	-w
Work, w	$-P\Delta V$	0	$nC_V\Delta T$	$-nRT\ln\left(rac{V_{ m f}}{V_{ m i}} ight)=-nRT\ln\left(rac{P_{ m i}}{P_{ m f}} ight)$
Energy, ΔE	q+w	q	$oldsymbol{w}$	0
Enthalpy, ΔH	q	$\Delta E + V \Delta P$	$V\Delta P$	0
Entropy, ΔS	$nC_{ m P} \ln \left(rac{T_{ m f}}{T_{ m i}} ight)$	$n C_{ m V} \ln \left(rac{T_{ m f}}{T_{ m i}} ight)$	0	$nR\ln\left(rac{V_{ m f}}{V_{ m i}} ight)=nR\ln\left(rac{P_{ m i}}{P_{ m f}} ight)$

4.3. The Adiabatic Condition

Given a rapid change in volume where q = 0, both P and T change to accommodate the compression or expansion.

$$\gamma = \frac{C_P}{C_V} = \frac{5}{3}$$

$$(P_1)(V_1)^{\gamma} = (P_2)(V_2)^{\gamma}$$

$$w = nC_V \Delta T$$

Temperature change in adiabatic compression or expansion:

$$T_{
m f} = T_{
m i} \left(rac{V_{
m i}}{V_{
m f}}
ight)^{(R/C_V)}$$

4.4. Enthalpy

Enthalpy is the energy required to create a system, plus the amount of energy required to make room for the system by displacing its environment by the system's volume at a given pressure.

$$H = E + PV$$

Enthalpy change for a reaction:

$$\Delta H = \Delta E + \Delta (PV) = \Delta E + P\Delta V + V\Delta P$$

Standard enthalpy of reaction, where n and m are coefficients in the balanced reaction equation:

$$\Delta H_{\rm rxn}^{\circ} = \sum n \Delta H_{\rm f}^{\circ}({\rm products}) - \sum m \Delta H_{\rm f}^{\circ}({\rm reactants}) = \sum D_{\rm broken} - \sum D_{\rm formed}$$

Clausius-Clapeyron equation:

$$\ln P = \frac{-\Delta H_{\text{vap}}}{RT} + C$$

Heat of vaporization based on the Clausius-Clapeyron equation:

$$\ln \frac{P_1}{P_2} = \frac{\Delta H_{\text{vap}}}{R} \left(\frac{1}{T_2} - \frac{1}{T_1} \right) = \frac{-\Delta H_{\text{vap}}}{R} \left(\frac{1}{T_1} - \frac{1}{T_2} \right)$$

4.5. Entropy

Second Law of Thermodynamics:

$$\Delta S_{\text{universe}} = \Delta S_{\text{system}} + \Delta S_{\text{surroundings}} > 0$$

Standard entropy of reaction, where n and m are coefficients in the balanced reaction equation:

$$\Delta S_{\rm rxn}^{\circ} = \sum n \Delta S^{\circ}(\text{products}) - \sum m \Delta S^{\circ}(\text{reactants})$$

Change in entropy with ΔH_{vap} or q where T is constant:

$$\Delta S = \frac{\Delta H_{\text{vap}}}{T} = \frac{q}{T}$$

Change in entropy with ΔV or ΔP where T is constant:

$$\Delta S = nR \ln \left(rac{V_{
m f}}{V_{
m i}}
ight) = nR \ln \left(rac{P_{
m i}}{P_{
m f}}
ight)$$

Change in entropy for a thermodynamic process where T and/or P are varied:

$$\Delta S = nC_V \ln \left(rac{T_{
m f}}{T_{
m i}}
ight) - nR \ln \left(rac{P_{
m f}}{P_{
m i}}
ight)$$

4.6. Gibbs Free Energy

Free energy change at constant temperature:

$$\Delta G^{\circ} = \Delta H^{\circ} - T \Delta S^{\circ}$$

Or for an equilibrium reaction:

$$\Delta G^{\circ} = -RT \ln K_{\rm eq}$$

Non-standard free energy:

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

Standard free energy of reaction, where n and m are coefficients in the balanced reaction equation:

$$\Delta G_{\rm rxn}^{\circ} = \sum n \Delta G_{\rm f}^{\circ}({\rm products}) - \sum m \Delta G_{\rm f}^{\circ}({\rm reactants})$$

5. Electromagnetism

Relationship of wavelength and frequency, where $c = 2.99 \times 10^8$ m/s:

$$c = \lambda \nu$$

Energy of a photon, where Planck's constant $h = 6.626 \times 10^{-34} \text{ J} \cdot \text{s}$:

$$E = h\nu = \frac{hc}{\lambda}$$

Energy of an electron in the $n^{\rm th}$ shell in a hydrogen atom, where $R_{\infty}=2.18\times 10^{-18}$ J:

$$E_n = Z^2 R_\infty \left(\frac{1}{n^2}\right)$$

Energy of a photon corresponding to an electron transition from the n_i shell to the n_f shell:

$$\Delta E = Z^2 R_{\infty} \left(rac{1}{n_{
m f}^2} - rac{1}{n_{
m i}^2}
ight)$$

Or, using $R_{\infty} = 10973731.6 \text{ m}^{-1}$:

$$rac{1}{\lambda} = Z^2 R_{\infty} \left(rac{1}{n_{
m f}^2} - rac{1}{n_{
m i}^2}
ight)$$

de Broglie wavelength; if the particle size is much smaller than λ , then quantum rules are needed:

$$\lambda = \frac{h}{mv}$$

Formal charge:

$$q_{\mathrm{F}} = N_i e_{\mathrm{V}} - N_i \mathrm{B} - N_k e_{\mathrm{NB}}$$

Dipole moment:

$$\mu = Q \times r$$

Bragg equation:

$$\lambda\nu = 2d\sin\theta$$

Coulomb's law, where $k_{\rm e}$ is Coulomb's constant $k_{\rm e}\approx 8.99\times 10^9~{\rm N\,m^2\,C^{-2}}$

$$F = k_{\rm e} \frac{q_1 q_2}{r^2}$$

cf. Newton's law of gravitation, where G is the universal gravitational constant, 6.674×10^{-11} m³ kg⁻¹ s⁻²

$$F = G \frac{m_1 m_2}{r^2}$$

6. Quantum Mechanics

Heisenberg Uncertainty Principle, Δx is the minimum "size of a box" for a particle:

$$\Delta x \Delta \rho \ge \frac{h}{4\pi}$$

The time-dependent Schrödinger equation:

$$i\hbar\frac{\partial}{\partial t}|\Psi(t)\rangle=\hat{H}|\Psi(t)\rangle$$

The time-independent Schrödinger equation for a particle of mass m moving in one direction with energy E where $\hbar = h/2\pi$ is:

$$-\frac{\hbar^2}{2m}\frac{d^2\Psi(x)}{dx^2} + V(x)\Psi(x) = E\Psi(x)$$

Wavefunction for the 1s orbital:

$$\psi_{1s} = \frac{1}{\sqrt{\pi}}e^{-r}$$

Wavefunction for the 2s orbital:

$$\psi_{2s} = \frac{1}{2\sqrt{2\pi}} \left(1 - \frac{r}{2} \right) e^{-r/2}$$

Wavefunction for the $2p_z$ orbital, where a_0 is the radius of the first Bohr orbit $(5.29 \times 10^{-11} \text{ m})$, $\sigma = Z(r/a_0)$ where r is the distance (in m) from the nucleus and Z is the nuclear charge, and θ is an angle:

$$\psi_{2p_z} = \frac{1}{4\sqrt{2\pi}} \left(\frac{Z}{a_0}\right)^{3/2} \sigma e^{-\sigma/2} \cos \theta$$

Wavefunction for a particle in a 1-dimensional box of length L:

$$\psi = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi}{L}\right) x$$

Energy for a particle in a 1-dimensional box of length L:

$$E = \frac{n^2 h^2}{8mL^2}$$

Potential energy between two charged bodies:

$$V = k \frac{q_1 q_2}{r}$$

7. Stoichiometry

Percent composition of an element in a compound, where n = the number of moles of the element in one mole of the compound:

$$\% = \left(\frac{n \times \text{molar mass of element}}{\text{molar mass of compound}}\right) \times 100\%$$

Percent yield:

% yield =
$$\left(\frac{\text{actual yield}}{\text{theoretical yield}}\right) \times 100\%$$

8. Electrochemistry

Electrical force between two charged bodies:

$$F_{e\ell} = k rac{q_1 q_2}{r_2}$$

Standard emf of an electrochemical cell F = 96485 coulomb/mol:

$$\mathscr{E}_{ ext{cell}}^{\circ} = \mathscr{E}_{ ext{ox}}^{\circ} - \mathscr{E}_{ ext{red}}^{\circ} = rac{RT}{nF} \ln K$$

Standard free energy of an electrochemical cell:

$$\Delta G^{\circ} = -nF\mathscr{E}_{\operatorname{cell}}^{\circ}$$

Nernst equation:

$$\mathscr{E}_{\text{cell}} = \mathscr{E}_{\text{cell}}^{\circ} - \frac{RT}{nF} \ln Q$$

Therefore: Standard free energy of an electrochemical cell:

$$\Delta G = -nF\mathscr{E}_{\text{cell}}$$

9. Reaction Kinetics

		Rate Laws	
Order	Standard Form	Integrated Form	Line Form
0	rate = k	$[\mathbf{A}]_t - [\mathbf{A}]_0 = -kt$	$[\mathbf{A}]_t = -kt + [\mathbf{A}]_0$
1	$\mathrm{rate} = k[\mathbf{A}]$	$\ln\frac{\left[\mathbf{A}\right]_t}{\left[\mathbf{A}\right]_0} = -kt$	$\ln \left[\mathbf{A} \right]_t = -kt + \ln \left[\mathbf{A} \right]_0$
2	$\mathrm{rate} = k[\mathbf{A}]^2$	$\frac{1}{[\mathrm{A}]_t} - \frac{1}{[\mathrm{A}]_0} = kt$	$\frac{1}{[A]_t} = kt + \frac{1}{[A]_0}$

Order	Half-life	Alternate Form
0	$t_{1/2}=rac{\left[\mathrm{A} ight]_0}{2k}$	
1	$t_{1/2}=rac{\ln 2}{k}$	$\ln rac{[\mathrm{A}]_t}{[\mathrm{A}]_0} = (-\ln 2) \left(rac{t}{t_{1/2}} ight)$
2	$t_{^1\!/_2}=rac{1}{k[{ m A}]_0}$	

Arrhenius equation:

$$k = A \exp \frac{-E_{\rm a}}{RT}$$
 and \ln form: $\ln k = \left(\frac{-E_{\rm a}}{R}\right) \left(\frac{1}{T}\right) + \ln A$

Relationships of rate constants at two different temperatures:

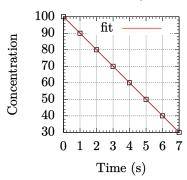
$$\ln \frac{k_1}{k_2} = \frac{E_a}{R} \left(\frac{1}{T_2} - \frac{1}{T_1} \right) = \frac{-E_a}{R} \left(\frac{1}{T_1} - \frac{1}{T_2} \right)$$

9.1. Kinetics Data

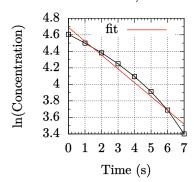
Table 3: Kinetics Data — 0th Order

Time	Concentration	ln(Concentration)	1/(Concentration)
0	100	4.605	0.0100
1	90	4.499	0.0110
2	80	4.382	0.0125
3	70	4.248	0.0141
4	60	4.094	0.0166
5	50	3.912	0.0200
6	40	3.688	0.0250
7	30	3.401	0.0333

0th Order Plot, $R^2 = 1$



1st Order Plot, $R^2 = 0.97$



2nd Order Plot, $R^2 = 0.89$

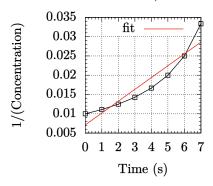
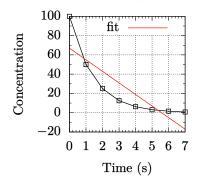


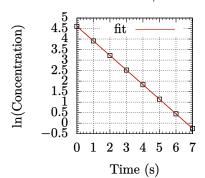
Table 4: Kinetics Data — 1st Order

Time	Concentration	ln(Concentration)	1/(Concentration)
0	100	4.605	0.01
1	50	3.912	0.02
2	25	3.218	0.04
3	12.5	2.525	0.08
4	6.25	1.832	0.16
5	3.13	1.141	0.32
6	1.56	0.444	0.64
7	0.78	-0.248	1.28

0th Order Plot, $R^2 = 0.73$



1st Order Plot, $R^2 = 1$



2nd Order Plot, $R^2 = 0.72$

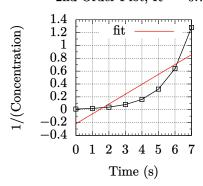
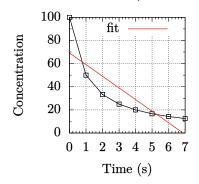


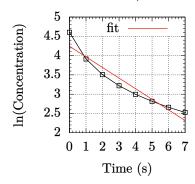
Table 5: Kinetics Data — 2nd Order

Time	Concentration	ln(Concentration)	1/(Concentration)
0	100	4.605	0.01
1	50	3.912	0.02
2	33.3	3.505	0.03
3	25	3.218	0.04
4	20	2.995	0.05
5	16.67	2.813	0.06
6	14.28	2.658	0.07
7	12.5	2.525	0.08

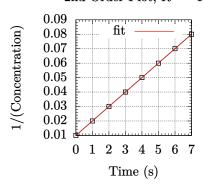
0th Order Plot, $R^2 = 0.70$



1st Order Plot, $R^2 = 0.92$



2nd Order Plot, $R^2 = 1$



10. Equilibrium

Law of Mass Action (equilibrium constant) for a reaction of form $aA + bB \longrightarrow cC + dD$:

$$K_{\text{eq}} = \frac{[\mathbf{C}]^c[\mathbf{D}]^d}{[\mathbf{A}]^a[\mathbf{B}]^b}$$

van't Hoff Equation

$$\ln\left(\frac{K_2}{K_1}\right) = \frac{-\Delta H^\circ}{R} \left(\frac{1}{T_2} - \frac{1}{T_1}\right) \text{ or } \ln K_{\rm sp} = \frac{-\Delta H^\circ}{RT} + \frac{\Delta S^\circ}{R}$$

Relationship between equilibrium constants for aqueous systems and for gases:

$$K_{\rm p} = K_{\rm c} R T^{\Delta n}$$

Ion product of water:

$$K_{\rm w} = [{\rm H_3O^+}][{\rm ^-OH}] = 1 \times 10^{-14}$$

10.1. Equilibrium of Acids and Bases

Definition of pH:

$$pH = -\log[H_3O^+]$$

Definition of pOH:

$$pOH = -\log[^-OH] = 14 - pH$$

For the reaction $HA + H_2O \longrightarrow H_3O^+ + A^-$:

$$K_{\rm a} = \frac{[{
m H_3O^+}][{
m A}^-]}{[{
m HA}]}$$

For the reaction $B + H_2O \longrightarrow BH^+ + {}^-OH$:

$$K_{\rm b} = \frac{[{\rm BH^+}][-{\rm OH}]}{[{\rm B}]}$$

Relationship between K_a , K_b , and K_w :

$$K_{\rm w} = K_{\rm a} K_{\rm b} = 1 \times 10^{-14}$$

Definition of pK_a :

$$pK_a = -\log(K_a)$$

Henderson-Hasselbalch equation:

$$pH = pK_a + \log \frac{[base]}{[acid]}$$

10.2. Equilibrium and Thermodynamics

Relationship between standard free-energy change and the equilibrium constant:

$$\Delta G^{\circ} = -RT \ln K$$

Non-standard free energy for a reaction of form $aA + bB \longrightarrow cC + dD$, where $Q = \frac{[C]^c[D]^d}{[A]^a[B]^b}$:

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

11. Similarity of Equations

11.1. Linear Equations with Different Temperatures

Clausius-Clapeyron Equation:

$$\ln \frac{P_1}{P_2} = \frac{\Delta H_{\text{vap}}}{R} \left(\frac{1}{T_2} - \frac{1}{T_1} \right) = \frac{-\Delta H_{\text{vap}}}{R} \left(\frac{1}{T_1} - \frac{1}{T_2} \right)$$

Arrhenius Equation:

$$\ln \frac{k_1}{k_2} = \frac{E_{\rm a}}{R} \left(\frac{1}{T_2} - \frac{1}{T_1} \right) = \frac{-E_{\rm a}}{R} \left(\frac{1}{T_1} - \frac{1}{T_2} \right)$$

van't Hoff Equation:

$$\ln\frac{K_1}{K_2} = \frac{\Delta H^\circ}{R} \left(\frac{1}{T_2} - \frac{1}{T_1}\right) = \frac{-\Delta H^\circ}{R} \left(\frac{1}{T_1} - \frac{1}{T_2}\right)$$

van't Hoff Equation with $K_{\rm sp}$ and entropy, plot $\ln K_{\rm sp}$ vs. 1/T:

$$\Delta H^{\circ} - T\Delta S^{\circ} = \Delta G^{\circ} = -RT \ln K_{\rm sp}$$

$$\ln K_{\rm sp} = \frac{-\Delta H^{\circ}}{RT} + \frac{\Delta S^{\circ}}{R}$$

11.2. Summations

Standard entropy of reaction, where n and m are coefficients in the balanced reaction equation:

$$\Delta S_{\rm rxn}^{\circ} = \sum n \Delta S^{\circ}({\rm products}) - \sum m \Delta S^{\circ}({\rm reactants})$$

Standard enthalpy of reaction, where n and m are coefficients in the balanced reaction equation:

$$\Delta H_{\rm rxn}^{\circ} = \sum n \Delta H_{\rm f}^{\circ}({\rm products}) - \sum m \Delta H_{\rm f}^{\circ}({\rm reactants})$$

Standard free energy of reaction, where n and m are coefficients in the balanced reaction equation:

$$\Delta G_{\rm rxn}^{\circ} = \sum n \Delta G_{\rm f}^{\circ}({\rm products}) - \sum m \Delta G_{\rm f}^{\circ}({\rm reactants})$$

12. Statistics

Arithmetic mean (average):

$$\overline{x} = \frac{\sum_{i} (x_i)}{n}$$

Standard deviation:

$$\sigma = \sqrt{\frac{\sum_{i}(x_{i} - \overline{x})^{2}}{n - 1}}$$

$$x_{i} \quad x_{i} - \overline{x} \quad (x_{i} - \overline{x})^{2} \quad \sum (x_{i} - \overline{x})^{2} \quad \sigma$$

$$0.685 \quad 0.003 \quad 0.000009$$

$$0.676 \quad -0.006 \quad 0.000036$$

$$0.669 \quad -0.013 \quad 0.000169$$

$$0.688 \quad 0.006 \quad 0.000036$$

$$0.692 \quad 0.010 \quad 0.000100$$

$$n = 5 \qquad 0.00035 \quad 0.0094$$

Confidence interval (true mean), see end of document for t values.

$$\mu = \overline{x} \pm \frac{t\sigma}{\sqrt{n}}$$

Outliers (Grubbs' Test): If $G > G_{ref}$ then x_i can be considered an outlier. See end of document for G values.

$$G = \frac{|x_i - \overline{x}|}{\sigma}$$

13. Other

Mass defect:

$$\Delta m = [Z(m_{\rm p} + m_{\rm e}) + (A - Z)m_{\rm n}] - m_{\rm atom}$$

Table 6: Values for mass defect equation.

Variable	Description	Value
Δm	mass defect	amu
$m_{ m p}$	mass of a proton	1.007277
$m_{ m n}$	mass of a neutron	1.008665
$m_{ m e}$	mass of an electron	0.000548597
$m_{ m atom}$	mass of nuclide	$_{Z}^{A}X$
Z	atomic number	number of protons
\boldsymbol{A}	mass number	number of nucleons

Relationship between mass defect and energy released:

$$\Delta E = (\Delta m)c^2$$

The Quadratic Formula: for a quadratic equation $ax^2 + bx + c = 0$, the solutions x are:

$$x = \frac{-b \pm \sqrt{b^2 - 4ac}}{2a}$$

14. Acidities

Acid	Conj. Base	$\mathrm{p}K_\mathrm{a}$	Remarks
HI	I-	-10	hydroiodic acid
HBr	${ m Br}^-$	-9	hydrobromic acid
$\mathrm{H_2SO_4}$	$\mathrm{HSO_4}^-$	-9	sulfuric acid
HCl	Cl^-	-7	hydrochloric acid
$\mathrm{H_{3}O^{+}}$	$\mathrm{H_{2}O}$	-2	hydronium
HNO_3	$\mathrm{NO_3}^-$	-1	nitric acid
HSO ₄ -	$\mathrm{SO_4}^{2-}$	2	$2^{\rm nd}$ H of sulfuric acid
$_{ m HF}$	\mathbf{F}^{-}	3	hydrofluoric acid
RCOOH	$RCOO^-$	4	carboxylic acids
$\mathrm{H_2S}$	HS^-	7	compare to H_2O
$\mathrm{NH_4}^+$	$\mathrm{NH_{3}}$	9	${f ammonium}$
HCN	NC^-	9.2	sp-hybridized carbanion
PhOH	PhO^{-}	10	$\mathrm{phenols}^a$
$\mathrm{H_2O}$	HO^-	15.7	water^b
ROH	RO^-	16	aliphatic alcohols c
$RC(O)NH_2$	$RC(O)NH^-$	17	amides
$RC(O)CH_3$	$RC(O)CH_2^-$	20	α -H of ketones
PhNH_2	$PHNH^-$	25	$\mathrm{aniline}^d$
$RC \equiv CH$	$RC \equiv C^-$	25	terminal alkyne $(sp H)$
${ m H_2}$	H^-	36	hydrogen gas
NH_3	$\mathrm{NH_2}^-$	38	ammonia
RNH_2	RNH^-	40	aliphatic amines

Footnotes:

A conjugate base can deprotonate any acid higher than it on this table.

15. Compound Units

- joule = $coulomb \times volt$
- joule = $kg \times m^2 / s^2$
- watt = joule / sec
- kilowatt = 1000 joules / sec
- kilowatt-hour = $(1000 \text{ joules / sec}) \times 3600 \text{ sec} = 3.6 \times 10^6 \text{ joules}$
- amp = coulomb / second
- 1000 milliamp-hour = 1 amp-hour = 3600 amp-seconds = 3600 coulombs

 $[^]a$ depending on the substitution of Ph, $\mathrm{p}K_\mathrm{a}$ can vary from 4–11

 $^{^{}b}$ water is amphoteric, so anything less acidic than water can act as a base in aqueous solution

 $[^]c$ depending on the substitution of R, p $K_{\rm a}$ can vary from 15–17

 $[^]d$ depending on the substitution of Ph, pKa can vary from 18–28

Standard Enthalpies of Formation & Standard Entropies of Common Compounds

Substance	State	$\Delta H_f^\circ ight(rac{\mathrm{kJ}}{\mathrm{mol}})$	$S^{\circ} \left(\frac{J}{\text{mol} \cdot K} \right)$	Substance	State	$\Delta H_f^{\circ} \over (rac{\mathrm{kJ}}{\mathrm{mol}})$	$S^{\circ} \left(\frac{J}{\text{mol} \cdot K} \right)$
Ag	S	0	42.6	$\overline{\text{Cl}_2}$	g	0	223.0
Ag^+	aq	105.79	72.7	Cl^-	aq	-167.080	56.5
AgCl	S	-127.01	96.2	${ m ClO_4}^-$	aq	-128.10	182.0
AgBr	S	-100.4	107.1	Cr	\mathbf{S}	0	23.8
$AgNO_3$	S	-124.4	140.9	$\mathrm{Cr_2O_3}$	g	-1139.7	81.2
Al	S	0	28.3	Cu	S	0	33.2
Al^{+3}	aq	-538.4	-321.7	$\mathrm{Cu^{+}}$	aq	+71.7	40.6
$AlCl_3$	\mathbf{S}	-704	110.7	Cu^{+2}	aq	+64.8	-99.6
Al_2O_3	\mathbf{S}	-1675.7	50.9	CuO	\mathbf{S}	-157.3	42.6
Ba	\mathbf{S}	0	62.8	Cu_2O	S	-168.6	93.1
$BaCl_2$	\mathbf{S}	-858.6	123.7	CuS	S	-53.1	66.5
$BaCO_3$	\mathbf{S}	-1216.3	112.1	Cu_2S	S	-79.5	120.9
$Ba(NO_3)_2$	\mathbf{S}	-992	214	CuSO_4	S	-771.4	107.6
BaO	\mathbf{S}	-553.5	70.4	F^-	aq	-335.35	-13.8
$Ba(OH)_2$	\mathbf{S}	-998.2	112	F_2	g	0	202.7
$BaSO_4$	\mathbf{S}	-1473.2	132.2	Fe	S	0	27.3
Br_2	ℓ	0	152.2	$Fe(OH)_3$	S	-823.0	106.7
\mathbf{C}	\mathbf{S}	0	5.7	$\mathrm{Fe_2O_3}$	S	-824.2	87.4
CCl_4	ℓ	-135.4	216.4	$\mathrm{Fe_3O_4}$	S	-1118.4	146.4
CHCl_3	ℓ	-134.5	201.7	H_2	g	0	130.6
CH_4	g	-74.8	186.2	H^{+}	aq	0	0.0^{*}
C_2H_2	g	+226.7	200.8	HBr	g	-36.29	198.6
C_2H_4	g	+52.3	219.5	$\mathrm{HCO_3}^-$	aq	-689.93	91.2
C_2H_6	g	-84.7	229.5	HCl	g	-92.31	186.8
C_3H_8	g	-103.8	269.9	$_{ m HF}$	g	-273.30	173.7
$\mathrm{CH_{3}OH}$	ℓ	-238.7	126.8	HI	g	26.50	206.5
C_2H_5OH	ℓ	-277.7	160.7	HNO_3	ℓ	-174.1	155.6
CO	g	-110.53	197.6	$\mathrm{HPO_4}^{-2}$	aq	-1299.0	-33.5
CO_2	g	-393.51	213.6	$\mathrm{HSO_4}^-$	aq	-886.9	131.8
${\rm CO_3}^{-2}$	aq	-675.23	-56.9	$\mathrm{H_{2}O}$	ℓ	-285.830	69.9
Ca	\mathbf{S}	0	41.4	$\mathrm{H}_2\mathrm{O}$	g	-241.826	188.7
Ca^{+2}	aq	-543.0	-53.1	$\mathrm{H_2PO_4}^-$	aq	-1302.6	90.4
$CaCl_2$	\mathbf{S}	-795.8	104.6	H_2S	g	-20.6	205.7
$CaCO_3$	\mathbf{S}	-1206.9	92.9	$_{ m Hg}$	ℓ	0	76.0
CaO	\mathbf{S}	-634.92	39.8	Hg^{+2}	aq	170.21	-32.2
$Ca(OH)_2$	S	-986.1	83.4	$_{ m HgO}$	$_{\rm cr,red}$	-90.79	70.3
$CaSO_4$	S	-1434.1	106.7				
Cd	\mathbf{S}	0	51.8				
Cd^{+2}	aq	-75.92	-73.2				
$CdCl_2$	\mathbf{S}	-391.5	115.3				
CdO	S	-258.35	54.8				

^{*}The standard entropy of the $\mathrm{H}^+(aq)$ ion is defined to be 0.

Substance	State	ΔH_f°	S° (J)
		$\left(\frac{\text{kJ}}{\text{mol}}\right)$	$\left(\frac{J}{\text{mol} \cdot K}\right)$
I-	aq	-56.78	111.3
I_2	S	0	116.1
K	S	0	64.2
K^{+}	aq	-252.14	102.5
KBr	S	-393.8	95.9
KCl	S	-436.7	82.6
$KClO_3$	S	-397.7	143.1
$KClO_4$	S	-432.8	151.0
KNO_3	S	-494.6	133.0
Mg	S	0	32.7
Mg^{+2}	aq	-467.0	-138.1
MgCl_2	\mathbf{S}	-641.3	89.6
$MgCO_3$	S	-1095.8	65.7
MgO	S	-601.60	26.9
$Mg(OH)_2$	\mathbf{S}	-924.5	63.2
$MgSO_4$	\mathbf{S}	-1284.9	91.6
Mn	S	0	32.0
$\mathrm{Mn^{+2}}$	aq	-220.8	-73.6
MnO	S	-385.2	59.7
MnO_2	S	-520.0	53.0
N_2	g	0	191.5
NH_3	g	-45.94	192.3
$\mathrm{NH_4}^+$	aq	-133.26	113.4
NO_2^-	aq	-104.6	123.0
NO_3^-	aq	-206.85	146.4
N_2H_4	ℓ	+50.6	121.2
$\mathrm{NH_4Cl}$	S	-314.4	94.6
NH_4NO_3	S	-365.6	151.1
NO	g	+90.2	210.7
NO_2	g	+33.2	240.0
N_2O_4	g	+9.2	304.2
Na	S	0	51.2
Na^{+}	aq	-240.34	59.0
NaCl	S	-411.2	72.1
NaF	S	-573.6	51.5
NaOH	S	425.6	64.5

Substance	State	ΔH_f°	$S^{\circ}_{_{_{\mathrm{J}}}}$	
		$\left(\frac{\mathrm{kJ}}{\mathrm{mol}}\right)$	$\frac{3}{\text{mol K}}$	
Ni	S	0	29.9	
NiO	\mathbf{S}	-239.7	38.0	
OH^-	aq	-230.015	-10.8	
O_2	g	0	205.0	
P_4	\mathbf{S}	0	164.4	
PCl_3	g	-287.0	311.7	
PCl_5	g	-374.9	364.5	
PO_4^{-3}	aq	-1277.4	-222	
Pb	\mathbf{S}	0	64.8	
Pb^{+2}	aq	0.92	10.5	
$PbBr_2$	\mathbf{S}	-278.7	161.5	
$PbCl_2$	\mathbf{S}	-359.4	136.0	
PbO	\mathbf{S}	-219.0	66.5	
PbO_2	\mathbf{S}	-277.4	68.6	
S	S	0	31.8	
SO_2	g	-296.81	248.1	
SO_3	g	-395.7	256.7	
SO_4^{-2}	aq	-909.34	20.1	
S_2^-	aq	+33.1	-14.6	
Si	S	0	18.8	
SiO_2	S	-910.7	41.8	
Sn	S	0	51.6	
Sn^{+2}	aq	-8.9	-17.4	
SnO_2	\mathbf{s}	-577.63	52.3	
Zn	\mathbf{s}	0	41.6	
Zn^{+2}	aq	-153.39	-112.1	
ZnI_2	\mathbf{s}	-208.0	161.1	
ZnO	\mathbf{s}	-350.46	43.6	
ZnS	\mathbf{s}	-206.0	57.7	

TABLE 9.3 Average Bond Energies

		Dona Li			
	Bond Energy		Bond Energy		Bond Energy
Bond	(kJ/mol)	Bond	(kJ/mol)	Bond	(kJ/mol)
н—н	436	N-N	163	Br—F	237
н—с	414	N=N	418	Br—Cl	218
H—N	389	N = N	946	Br—Br	193
н—о	464	N-O	222	I—CI	208
H—S	368	N=0	590	I—Br	175
H—F	565	N-F	272	I—I	151
H—CI	431	N—CI	200	Si—H	323
H—Br	364	N—Br	243	Si—Si	226
H—I	297	N—I	159	si-c	301
с—с	347	0-0	142	s-0	265
c=c	611	0=0	498	Si=0	368
C≡C	837	0—F	190	s=0	523
c-N	305	o—cı	203	Si—Cl	464
C=N	615	0—I	234	s=s	418
C≡N	891	F—F	159	S-F	327
o	360	CI-F	253	s-cı	253
c=0	736*	cı—cı	243	S—Br	218
C≡O	1072			s-s	266
C—CI	339				

^{*799} in CO₂

TABLE 10.4 Van der Waals Constants for Common Gases

Gas	a (L² · atm/mol²)	b (L/mol)
He	0.0342	0.02370
Ne	0.211	0.0171
Ar	1.35	0.0322
Kr	2.32	0.0398
Xe	4.19	0.0511
H ₂	0.244	0.0266
N ₂	1.39	0.0391
O ₂	1.36	0.0318
CI ₂	6.49	0.0562
H ₂ O	5.46	0.0305
CH ₄	2.25	0.0428
CO ₂	3.59	0.0427
CCI ₄	20.4	0.1383

Values of Grubbs Statistic (G)

	Confidence Level (%)								
Number of Observations n	99.9	99.5	99	97.5	95	90			
3	1.155	1.155	1.155	1.155	1.153	1.148			
4	1.499	1.496	1.492	1.481	1.463	1.425			
5	1.780	1.764	1.749	1.715	1.672	1.602			
6	2.011	1.973	1.944	1.887	1.822	1.729			
7	2.201	2.139	2.097	2.020	1.938	1.828			
8	2.358	2.274	2.221	2.126	2.032	1.909			
9	2.492	2.387	2.323	2.215	2.110	1.977			
10	2.606	2.482	2.410	2.290	2.176	2.036			
11	2.705	2.564	2.485	2.355	2.234	2.088			
12	2.791	2.636	2.550	2.412	2.285	2.134			
13	2.867	2.699	2.607	2.462	2.331	2.175			
14	2.935	2.755	2.659	2.507	2.371	2.213			
15	2.997	2.806	2.705	2.549	2.409	2.247			
16	3.052	2.852	2.747	2.585	2.443	2.279			
17	3.103	2.894	2.785	2.620	2.475	2.309			
18	3.149	2.932	2.821	2.651	2.504	2.335			
19	3.191	2.968	2.854	2.681	2.532	2.361			
20	3.230	3.001	2.884	2.709	2.557	2.385			
30	3.507	3.236	3.103	2.908	2.745	2.563			
40	3.673	3.381	3.240	3.036	2.866	2.682			
50	3.789	3.483	3.336	3.128	2.956	2.768			
60	3.874	3.560	3.411	3.199	3.025	2.837			
70	3.942	3.622	3.471	3.257	3.082	2.893			
80	3.998	3.673	3.521	3.305	3.130	2.940			
90	4.044	3.716	3.563	3.347	3.171	2.981			
100	4.084	3.754	3.600	3.383	3.207	3.017			

Source: ASTM E178-00, "Standard Practice for Dealing with Outlying Observations"

Values of Student's t

	Confidence Level (%)									
Degrees of Freedom	50	90	95	97.5	99	99.5	99.9			
1	1.000	6.314	12.706	25.452	63.657	127.321	636.619			
2	0.816	2.920	4.303	6.205	9.925	14.089	31.599			
3	0.765	2.353	3.182	4.177	5.841	7.453	12.924			
4	0.741	2.132	2.776	3.495	4.604	5.598	8.610			
5	0.727	2.015	2.571	3.163	4.032	4.773	6.869			
6	0.718	1.943	2.447	2.969	3.707	4.317	5.959			
7	0.711	1.895	2.365	2.841	3.499	4.029	5.408			
8	0.706	1.860	2.306	2.752	3.355	3.833	5.041			
9	0.703	1.833	2.262	2.685	3.250	3.690	4.781			
10	0.700	1.812	2.228	2.634	3.169	3.581	4.587			
11	0.697	1.796	2.201	2.593	3.106	3.497	4.437			
12	0.695	1.782	2.179	2.560	3.055	3.428	4.318			
13	0.694	1.771	2.160	2.533	3.012	3.372	4.221			
14	0.692	1.761	2.145	2.510	2.977	3.326	4.140			
15	0.691	1.753	2.131	2.490	2.947	3.286	4.073			
16	0.690	1.746	2.120	2.473	2.921	3.252	4.015			
17	0.689	1.740	2.110	2.458	2.898	3.222	3.965			
18	0.688	1.734	2.101	2.445	2.878	3.197	3.922			
19	0.688	1.729	2.093	2.433	2.861	3.174	3.883			
20	0.687	1.725	2.086	2.423	2.845	3.153	3.850			
30	0.683	1.697	2.042	2.360	2.750	3.030	3.646			
40	0.681	1.684	2.021	2.329	2.704	2.971	3.551			
50	0.679	1.676	2.009	2.311	2.678	2.937	3.496			
60	0.679	1.671	2.000	2.299	2.660	2.915	3.460			
70	0.678	1.667	1.994	2.291	2.648	2.899	3.435			
80	0.678	1.664	1.990	2.284	2.639	2.887	3.416			
90	0.677	1.662	1.987	2.280	2.632	2.878	3.402			
100	0.677	1.660	1.984	2.276	2.626	2.871	3.390			
∞	0.674	1.645	1.960	2.241	2.576	2.807	3.291			

Values for the F Statistic at the 95% Confidence Level

	Degrees of Freedom (numerator)										
Degrees of Freedom (denominator)	2	3	4	5	6	7	8	9	10	20	∞
2	19.00	19.16	19.25	19.30	19.33	19.35	19.37	19.38	19.40	19.45	19.50
3	9.55	9.28	9.12	9.01	8.94	8.89	8.85	8.81	8.79	8.66	8.53
4	6.94	6.59	6.39	6.26	6.16	6.09	6.04	6.00	5.96	5.80	5.63
5	5.79	5.41	5.19	5.05	4.95	4.88	4.82	4.77	4.74	4.56	4.36
6	5.14	4.76	4.53	4.39	4.28	4.21	4.15	4.10	4.06	3.87	3.67
7	4.74	4.35	4.12	3.97	3.87	3.79	3.73	3.68	3.64	3.44	3.23
8	4.46	4.07	3.84	3.69	3.58	3.50	3.44	3.39	3.35	3.15	2.93
9	4.26	3.86	3.63	3.48	3.37	3.29	3.23	3.18	3.14	2.94	2.71
10	4.10	3.71	3.48	3.33	3.22	3.14	3.07	3.02	2.98	2.77	2.54
20	3.49	3.10	2.87	2.71	2.60	2.51	2.45	2.39	2.35	2.12	1.84
	3.00	2.60	2.37	2.21	2.10	2.01	1.94	1.88	1.83	1.57	1.00

Values for the F Statistic at the 90% Confidence Level

	Degrees of Freedom (numerator)										
Degrees of Freedom (denominator)	2	3	4	5	6	7	8	9	10	20	∞
2	9.00	9.16	9.24	9.29	9.33	9.35	9.37	9.38	9.39	9.44	9.49
3	5.46	5.39	5.34	5.31	5.28	5.27	5.25	5.24	5.23	5.18	5.13
4	4.32	4.19	4.11	4.05	4.01	3.98	3.95	3.94	3.92	3.84	3.76
5	3.78	3.62	3.52	3.45	3.40	3.37	3.34	3.32	3.30	3.21	3.10
6	3.46	3.29	3.18	3.11	3.05	3.01	2.98	2.96	2.94	2.84	2.72
7	3.26	3.07	2.96	2.88	2.83	2.78	2.75	2.72	2.70	2.59	2.47
8	3.11	2.92	2.81	2.73	2.67	2.62	2.59	2.56	2.54	2.42	2.29
9	3.01	2.81	2.69	2.61	2.55	2.51	2.47	2.44	2.42	2.30	2.16
10	2.92	2.73	2.61	2.52	2.46	2.41	2.38	2.35	2.32	2.20	2.06
20	2.59	2.38	2.25	2.16	2.09	2.04	2.00	1.96	1.94	1.79	1.61
∞	2.30	2.08	1.94	1.85	1.77	1.72	1.67	1.63	1.60	1.42	1.00