Data Sheet – BCH341 – BioPchem – Tinoco

Useful Equations & Mathematical Relations:

$F_{sp} = -F_{ex} = -k(x-x_o)$

$w = \int F_{ex}(x)\ dx = \int -k(x - x_o)\, dx$

$$w = \int F_{ex}(x)\ dx = \int mg\, dx \approx mg \int dx = mgh$$

$PV = nRT$

Pressure=F/A = gm/A

$P_i = \chi_i P_T$

$dq = Cdt$

$\chi_i = \frac{n_i}{\sum_i n_i}$

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

$w = -nRT\ ln\left({V_2}/{V_1}\right)$

$\Delta U = q + w$

$dU = \partial q + \partial w$

$H \equiv U + PV$

$C_V = \left(\frac{\partial U}{\partial T}\right)_V$

$C_P = \left(\frac{\partial H}{\partial T}\right)_P$

$dH = C_P dT$

$\Delta H = nC_P \Delta T$

$C_V = {3}/{2}\, R$

$C_P - C_V = R$

$P_1 V_1 = P_2 V_2$

$w = nC_V \Delta T$

$\Delta_r H^o\ (T') = \Delta_r H^o\ (T) + \Delta_r C_P^o\ (T'-T)$

$\Delta_r H^o = \sum \nu \Delta_f H^o$ (products) - $\sum \nu \Delta_f H^o$ (reactants)

$\Delta_r C_P^o = \sum \nu C_p^o$ (products) - $\sum \nu C_p^o$ (reactants)

$\Delta_r S^o = \sum \nu S_m^o$ (products) - $\sum \nu S_m^o$ (reactants)

$\Delta_r G^o = \sum \nu G_m^o$ (products) - $\sum \nu G_m^o$ (reactants)

$S = k_B lnW$

$\Delta S = nR\ ln\left(\frac{V_2}{V_1}\right)$

$\Delta S = \frac{q_{rev}}{T}$

$dS = \frac{dq_{rev}}{T}$

$\Delta S_{univ} = \Delta S_{sys} + \Delta S_{surr} \geq 0$

$\Delta S_{mix} = -nR(\chi_A ln\ \chi_A + \chi_B ln\ \chi_B)$

$\Delta_{fus} S = \frac{\Delta_{fus} H}{T_{fus}}$

$\Delta_{vap} S = \frac{\Delta_{vap} H}{T_{b.p.}}$

$\Delta S = nC_P\ ln\left({T_2}/{T_1}\right)$

$G \equiv U + PV - TS = H - TS$

$\Delta G = \Delta H - T\Delta S$

$dU = TdS - PdV$

$dG = VdP - SdT$

$\Delta G = nRT\ ln\left({P_2}/{P_1}\right)$

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

$G_i = \left(\frac{\partial G}{\partial n_i}\right)_{T,P,n_{i\neq i}}$

$G_i = \mu_i$

Work=force x distance

$P = \rho gh$

$\rho = m/V$

$F = ma$

$E_K = 1/2 mv^2$

$w = -P_{ex}\Delta V$

q = heat = $C\Delta T$

$\Delta H = \Delta U + \Delta(PV)$

$\Delta U = w + q$ $\quad$ $dU = dq + dw = TdS - PdV$

$dS \geq q/T$ (most general statement of the 2nd law)

$\Delta G = nG_m(2) - nG_m(1)$ $\quad$ $\Delta G_{mix} = nRT(\chi_A \ln \chi_A + \chi_B \ln \chi_B)$

$\chi_j = n_j/n$ $\quad$ $P_j = \chi_j P$

$M = \rho RT/P$ $\quad$ $P_B = \chi_B K_B$

$\Delta_r G = \Delta_r G^\theta + RT \ln Q$ $\quad$ $\Delta_r G^\theta = -RT \ln K$

$\Delta_r G^o = \Delta_r H^o - T\Delta_r S^o$ $\quad$ $\Delta G^o = -RT\, lnK_P$

$\Delta_r G^\theta = \sum \nu G_m^o$ (products) - $\sum \nu G_m^o$ (reactants)

$\Delta G = \Delta G^o + RT\, lnQ$ $\quad$ $ln\left({}^{K_2}/_{K_1}\right) = -\frac{\Delta_r H^o}{R}\left({}^1/_{T_2} - {}^1/_{T_1}\right)$

$\left[\frac{\partial ln(K)}{\partial(1/T)}\right]_P = -\frac{\Delta_r H^o}{R}$ $\quad$ $\mu_A = \mu_A^o + RTlna_A$

$pH = pK_A + log\frac{c_S}{c_A}$ $\quad$ $\log \gamma_i = -0.509 Z_i^2 \sqrt{I}$

$I = \frac{1}{2}\sum_i c_i Z_i^2$ $\quad$ $\frac{N_i}{N} = \frac{g_i e^{-E_i/k_B T}}{Q}$

$Q = \sum_i g_i e^{-E_i/k_B T} = partion\ function$ $\quad$ $S = k \ln W$

$\langle h^2 \rangle = Nl^2$ $\quad$ $\langle R^2 \rangle = \frac{Nl^2}{6}$ (open-ended random coil)

$\langle R^2 \rangle = \frac{Nl^2}{12}$ (circular random coil) $\quad$ $\frac{\nu}{[A]} = k(N - \nu)$

$\frac{f}{1-f} = K[A]$ $\quad$ $\frac{d \log[\frac{f}{1-f}]}{d \log[A]} = N$

$F = C - P + 2$ $\quad$ $\lim_{\chi_A \to 1}\left(\frac{P_{vap}}{P_{vap}^o}\right) = \chi_A$

$\mu = \mu^o + RT \ln P_{vap}$ $\quad$ $\mu = \mu^o + RT \ln\left(\frac{P_{vap}}{P^o}\right)$

$\mu_A = \mu_A^o + RT \ln \chi_A$ $\quad$ $\Pi = \frac{RT}{V} n_B = cRT = \frac{w}{M} RT$

$T_f^o - T_f = K_f m$ $\quad$ $T_b - T_b^o = K_b m$

$\mu_A = \mu_A^o + RT \ln a_{xA}$ $\quad$ $a_{xA} = \gamma_A \chi_A$

$\Delta G = QV_{ex} = w_e$ $\quad$ $\Delta G^o = -\nu_e F \mathcal{E}^o$

$\mathcal{E} = \mathcal{E}^o - \frac{RT}{\nu_e F} lnQ$ $\quad$ $\mathcal{E}^o = \frac{RT}{\nu_e F} lnK$

$\Delta\mu = \Delta\mu_E + \Delta\mu_C = ZFV + RTlnQ$ $\quad$ $V = -(RT/ZF)lnK$

$z = N_A p \pi d^2 \sqrt{\frac{16}{\pi RTM}} = N_A p \sigma \sqrt{\frac{16}{\pi RTM}}$ $\quad$ $\lambda = \frac{RT}{\sqrt{2} N_A p \sigma}$

$\langle d^2 \rangle = \langle \nu \rangle \lambda t = \frac{2(RT)^{3/2} t}{\sqrt{M\pi} N_A p \sigma}$ $\quad$ $J_x = -D\left(\frac{dc}{dx}\right)$

$\left(\frac{dc}{dt}\right)_x = D\left(\frac{d^2 c}{dx^2}\right)_t$ $\quad$ $D = \frac{k_B T}{f}$

$$f = 6\pi\eta r$$

$$s = \frac{\nu_t}{g} = \frac{m_B(1-\nu_B\rho_A)}{f}$$

One dimension:

$$\langle d^2 \rangle = 2Dt$$

Three dimensions:

$$\langle d^2 \rangle = 6Dt$$

$$s_{20,w} = s\left(\frac{\eta}{\eta_{20,w}}\right)\frac{(1-\nu_B\rho_A)_{20,w}}{(1-\nu_B\rho_A)}$$

$$r = \left(\frac{3V_B}{4\pi}\right)^{1/3} = \left(\frac{3m_B\nu_B}{4\pi}\right)^{1/3}$$

$$f_0 = 6\pi\eta\left(\frac{3m_B\nu_B}{4\pi}\right)^{1/3}$$

$$M_B = \frac{RTs}{D(1-\nu_B\rho_A)}$$

$$\mu = \frac{\nu_t}{E}$$

$$\nu_t = \frac{ZeE}{f}$$

$$logM = a + bx$$

$$k = A\,exp\left(-\frac{E_a}{RT}\right)$$

$$\frac{dc}{dt} = -k$$ zero-order rxn

$$c_2 - c_1 = -k(t_2 - t_1)$$

$$\frac{dc}{dt} = -k\,c$$ first-order rxn

$$ln\frac{c_2}{c_1} = -k(t_2 - t_1)$$

$$\frac{dc}{dt} = -k\,c^2$$ second-order rnx (class I)

$$\frac{1}{c} = kt + \frac{1}{c_0}$$

$$\frac{dc}{dt} = -k\,c_A c_B$$ second-order rnx (class II)

$$t_{1/2} = \frac{ln2}{k}$$ first-order rxn

$$E_a = \frac{RT_2T_1}{T_2 - T_1}ln\frac{k_2}{k_1}$$

$$k = \frac{k_BT}{h}exp\left(\frac{\Delta S^\ddagger}{R}\right)exp\left(-\frac{\Delta H^\ddagger}{R}\right)$$

$$\Delta H^\ddagger = E_a - RT \approx E_a$$

$$\Delta S^\ddagger \approx R\left(ln\frac{Ah}{k_BT}\right)$$

$$\nu = k'[E]$$ enzyme concentration

$$\nu = k''[S]$$ substrate concentration

$$k_{cat} = \frac{V_{max}}{n[E]_o}$$

$$\nu_o = \frac{V_{max}[S]}{K_M + [S]}$$

$$\frac{1}{\nu_o} = \frac{1}{V_{max}} + \frac{K_M}{V_{max}}\frac{1}{[S]}$$

Conversion Factors:

1 N = 1 kg m s^{-2}

1 Pa = 1 kg m^{-1} s^{-2} = N / m^2

$1\ J = N\ m = 1\ kg\ m^2\ s^{-2}$	$1\ bar \approx 1\ atm$
$1\ atm = 760\ torr$	$1\ atm = 760\ mm\ Hg$
$T(K)=T(^oC)+273.15$	$R = 0.08206\ atm(L)/mol(K) = 8.3145\ J\ mol^{-1}\ K^{-1}$
$k_B=1.38x10^{-23}\ J/K$	$1\ L\ atm = 101.34\ J$
$1L = 1x10^{-3}\ m^3$	$N_A = 6.02214x10^{23}$
$1\ bar = 1x10^5\ Pa$	$1\ cal = 4.184\ J$
$F = 96485\ C/mol$	$c = 2.998x10^8\ m/s$
$RT/F = 25.693\ mV$	$1\ eV = 8065.5\ cm^{-1}$
$e = 2.71828$	$\pi = 3.14159$
$e = 1.6x10^{-19}\ C$	$h = 6.626x10^{-34}\ J\ s$
$\varepsilon_o = 8.854x10^{-12}\ C^2/J\ m$	A = 0.509 (water, Debye-Huckel constant)
$g = 9.8\ m/s^2$	1 Amp = 1 A = 1 C/s (Coulomb per sec)

Mathematical Relationships:

$\ln x = \ln 10 * \log x \approx 2.3 \log x$

$\ln x + \ln y = \ln xy$	$\ln x - \ln y = \ln(x/y)$
$d \ln x / dx = 1/x$	$d(f+g) = df + dg$
$d(fg) = f dg + g df$	$d(f/g) = 1/g\ df = f/g^2\ dg$
$\int x^n\ dx = (x^{n+1}) / (n+1) + \text{constant}$	$\int 1/x = \ln x + \text{constant}$
$\ln N! = N \ln N – N$	

TABLE 7.1 Standard Reduction Electrode Potentials at 25°C

Oxidant/Reductant	Electrode reaction	$\mathcal{E}°$(V)	$\mathcal{E}°'$(V) (pH 7)
K^+/K	$K^+ + e^- \rightarrow K$	–2.931	
Ca^{2+}/Ca	$Ca^{2+} + 2e^- \rightarrow Ca$	–2.868	
Na^+/Na	$Na^+ + e^- \rightarrow Na$	–2.71	
Mg^{2+}/Mg	$Mg^{2+} + 2e^- \rightarrow Mg$	–2.372	
Mn^{2+}/Mn	$Mn^{2+} + 2e^- \rightarrow Mn$	–1.185	
Zn^{2+}/Zn	$Zn^{2+} + 2e^- \rightarrow Zn$	–0.7618	
Acetate/acetaldehyde	$CH_3COO^- + 2e^- + 3H^+ \rightarrow CH_3CHO + H_2O$	–0.105	–0.586
Fe^{2+}/Fe	$Fe^{2+} + 2e^- \rightarrow Fe$	–0.447	
$H^+/H_2/Pt$	$2H^+ + 2e^- \rightarrow H_2$	0	–0.414
CO_2/formate	$CO_2(aq) + H^+ + 2e^- \rightarrow HCOO^-$	–0.181	–0.409
Ferredoxin	$Fd[Fe^{3+}] \rightarrow Fd[Fe^{2+}]$		–0.395
FMN(Mitochondrial complex I)	$FMN + 2H^+ + 2e^- \rightarrow FMNH_2$		–0.380
Gluconolactone/glucose	$C_6H_{10}O_6 + 2H^+ + 2e^- \rightarrow C_6H_{12}O_6$		–0.345
L-cystine/L-cysteine	L-cystine $+ 2H^+ + 2e^- \rightarrow$ 2 L-cysteine		–0.355
Fe^{3+}/Fe	$Fe^{3+} + 2e^- \rightarrow Fe$	–0.037	
Acetoacetate/ β-hydroxybutyrate	$CH_3COCH_2COO^- + 2H^+ + 2e^- \rightarrow CH_3CHOHCH_2COO^-$		–0.346
$NADP^+/NADPH$	$NADP^+ + H^+ + 2e^- \rightarrow NADPH$		–0.339
$NAD^+/NADH$	$NAD^+ + H^+ + 2e^- \rightarrow NADH$		–0.324
Glutathione(S-S)/ GlutathioneSH	$GSSG + 2H^+ + 2e^- \rightarrow 2\,GSH$		–0.240
$FMN/FMNH_2$	$FMN + 2H^+ + 2e^- \rightarrow FMNH_2$		–0.213
$FAD/FADH_2$	$FAD + 2H^+ + 2e^- \rightarrow FADH_2$		–0.212
Acetaldehyde/ethanol	$CH_3CHO + 2e^- + 2H^+ \rightarrow CH_3CH_2OH$	+0.221	–0.193
Pyruvate/lactate	$CH_3COCOO^- + 2H^+ + 2e^- \rightarrow CH_3CHOHCOO^-$		–0.184
Oxaloacetate/malate	$^-OOCCOCH_2COO^- + 2H^+ + 2e^- \rightarrow {}^-OOCCHOHCH_2COO^-$		–0.158
$FAD/FADH_2$(Complex II)	$FAD^+ + 2H^+ + 2e^- \rightarrow FADH_2$		–0.05
Fumarate/succinate	$^-OOCCH{=}CHCOO^- + 2H^+ + 2e^- \rightarrow {}^-OOCCH_2CH_2COO^-$		+0.045
Myoglobin	$Mb[Fe^{3+}] + e^- \rightarrow Mb[Fe^{2+}]$		+0.046
Ubiquinone	$UQ + 2H^+ + 2e^- \rightarrow UQH_2$		+0.052
Dehydroascorbate/ ascorbate	$DHA + H^+ + 2e^- \rightarrow Asc^-$		+0.080
$AgCl/Ag/Cl^-$	$AgCl + e^- \rightarrow Ag + Cl^-$	+0.222	
Cytochrome *c*	$Cyt\text{-}c[Fe^{3+}] + e^- \rightarrow Cyt\text{-}c[Fe^{2+}]$		+0.254
Calomel	$\frac{1}{2}Hg_2Cl_2 + e^- \rightarrow Hg + Cl^-$	+0.268	
O_2/H_2O_2	$O_2 + 2H^+ + 2e^- \rightarrow H_2O_2$	+0.695	+0.281

TABLE 7.1 Standard Reduction Electrode Potentials at 25°C *(cont.)*

Oxidant/Reductant	Electrode reaction	$\mathcal{E}°$(V)	$\mathcal{E}°'$(V) (pH 7)
Cu^{2+}/Cu	$Cu^{2+} + 2e^- \rightarrow Cu$	+0.342	
I_2/I^-	$I_2 + 2e^- \rightarrow 2\,I^-$	+0.535	
Ag^+/Ag	$Ag^+ + e^- \rightarrow Ag$	+0.800	
O_2/H_2O	$O_2 + 4H^+ + 4e^- \rightarrow 2H_2O$	+1.229	+0.815
NO_3^-/NO_2^-	$NO_3^- + 3H^+ + 2e^- \rightarrow HNO_2 + H_2O$	+0.934	
$Br_2(aq)/Br^-$	$Br_2 + 2e^- \rightarrow 2Br^-$	+1.087	
$Cl_2(g)/Cl^-$	$Cl_2 + 2e^- \rightarrow 2Cl^-$	+1.358	
Mn^{3+}/Mn^{2+}	$Mn^{3+} + e^- \rightarrow Mn^{2+}$	+1.541	
$F_2(g)/F^-$	$F_2 + 2e^- \rightarrow 2F^-$	+2.866	

TABLE 9.1 Rate Laws and Kinetic Order for Some Reactions

Stoichiometric reaction	Rate law	Kinetic order
sucrose + $H_2O \longrightarrow$ fructose + glucose	$v = k$[sucrose]	1
L-isoleucine $\longrightarrow$ D-isoleucine	$v = k$[L-isoleucine]	1
$^{14}C \longrightarrow {}^{14}N + \beta^-$	$v = k[^{14}C]$	1
2 proflavin $\longrightarrow$ proflavin dimer	$v = k[\text{proflavin}]^2$	2
p-nitrophenylacetate + 2 $OH^- \longrightarrow$ *p*-nitrophenolate + acetate + H_2O (pH 9)	$v = k[p\text{-nitrophenylacetate}][OH^-]$	2 (overall)
hemoglobin·$3O_2 + O_2 \longrightarrow$ hemoglobin·$4O_2$	$v = k[\text{Hb}\cdot 3O_2][O_2]$	2 (overall)
$H_2 + I_2 \longrightarrow 2\,HI$	$v = k[H_2][I_2]$	2 (overall)
$H_2 + Br_2 \longrightarrow 2\,HBr$	$v = \dfrac{k[H_2][Br_2]^{1/2}}{k' + [HBr]/[Br_2]}$	Complex
$CH_3CHO \longrightarrow CH_4 + CO$	$v \cong [CH_3CHO]^{3/2}$	3/2 (approx.)
$C_2H_5OH \longrightarrow CH_3CHO$ (liver enzymes)	v constant	0

TABLE 8.1 Transport and Related Properties of Some Proteins

	$s_{20,w}$ (S)	$D_{20,w} \times 10^{11}$ ($m^2\,s^{-1}$)	$\bar{v}_B$ ($mL\,g^{-1}$)	M_B	f/f_0
Ferricytochrome c (bovine heart)	1.91	13.20	0.707	12,744	1.077
Ribonuclease (bovine pancreas)	2.00	13.10	0.707	13,690	1.066
Myoglobin (horse heart)	2.04	11.30	0.741	16,951	1.105
Lysozyme (chicken egg white)	1.91	11.20	0.703	14,314	1.210
Chymotrypsinogen (bovine pancreas)	2.54	9.50	0.721	25,666	1.193
Immunoglobulin G (human)	6.6 − 7.2	4.00	0.739	156,000	1.513
Myosin	6.4	1.1	0.728	570,000	3.6
Tobacco mosaic virus	192	0.44	0.73	40,000,000	2.6

Sources: Based on data from Cantor and Schimmel (1980), Andrews, A. T. (1986), Chang, R. (2000), Harding, S. E., A. J. Rowe, and J. C. Horton, eds. (1992), Schuster, T. M. A., and T. M. Laue, eds. (1994), Van Holde, K. E., W. C. Johnson, and P. S. Ho. (1998) and Celis, J. D., and R. Bravo, eds. (1984).

		$[\eta]$, mL g^{-1}	
Protein	***M***	**normal**	**unfolded**
Ribonuclease (cow)	13,690	3.3	16.6
Myoglobin (horse)	17,568	3.1	20.9
Chymotrypsinogen(cow)	25,666	2.5	26.8
Serum albumin (cow)	66,296	3.7	52.2

Liquid	D, m^2s^{-1}
n-C_5H_{12}	5.6×10^{-9}
CH_3OH	2.6×10^{-9}
C_2H_5OH	1.2×10^{-9}
glycerol	2.5×10^{-12}

Protein	M (kD)	D, m^2s^{-1}
lysozyme	14.3	1.1×10^{-10}
5S-rRNA	40	5.9×10^{-11}
hemoglobin	68	7.0×10^{-11}
TMV	40800	4.5×10^{-12}

Macromolecule	v_B (mL g^{-1})
protein	0.69 − 0.75
starch	0.601
DNA	0.54
RNA	0.53

Protein	v_B (mL g^{-1})
lysozyme	0.742
serum albumin	0.735
lactalbumin	0.735
ribonuclease	0.700
hemoglobin	0.748

TABLE 10.2 Catalytic Constants for Several Enzymes

Enzyme	Substrate	Catalytic constant, k_{cat} (s^{-1})	Reference*
Catalase	H_2O_2	9×10^6	a
Acetylcholinesterase	Acetylcholine	1.2×10^4	b
Lactate dehydroge-nase (chicken)	Pyruvate	6×10^3	c
Chymotrypsin	Acetyl-L-tyrosine ethyl ester	4.3×10^2	d
Myosin	ATP	3	e
Fumarase	L-malate fumarate	1.1×10^3 2.5×10^3	f
Carbonic anhydrase (bovine)	CO_2 HCO_3^-	8×10^4 3×10^4	g

TABLE 9.3 The Characteristics of Simple-Order Reactions

Reaction order	Linear plot	Rate proportional to	Units of k
Zero-order	c vs t	$dc/dt = -k$	M s^{-1}
First-order	ln c vs. t	$dc/dt = -kc$	s^{-1}
Second-order (I)	$1/c$ vs t	$dc/dt = -kc^2$	M^{-1} s^{-1}
nth-order	$1/c^{n-1}$ vs t	$dc/dt = -kc^n$	$M^{-(n-1)}$ s^{-1}