

H⁺ Consumption and Release Stoichiometry

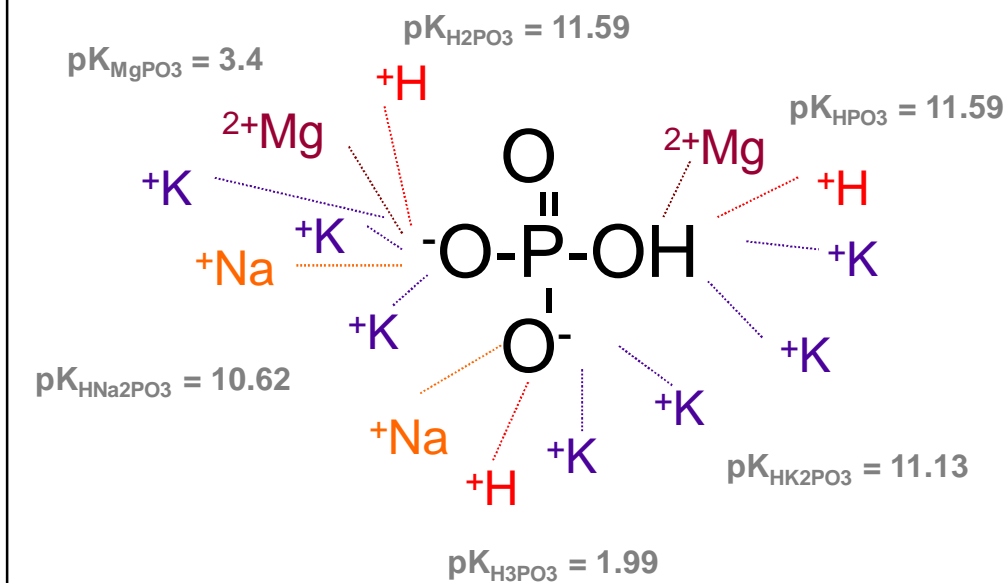
H⁺ binding or release are not singular during chemical reactions involving H⁺ as substrates or products.

To understand H⁺ balance during chemical reactions, fractional H⁺ binding must be understood and computed.

Accurate computations of fractional H⁺ binding require adjustments for competitive binding of metabolites with other cations.

UNM

Competitive Cation Binding



UNM

Methods

Latest electronic version of the NIST data base.

pK_{L-M^+} data were identified for as many metabolite cation complexes of non-mitochondrial energy metabolism as possible.

Data not in the NIST data base were obtained from prior research.

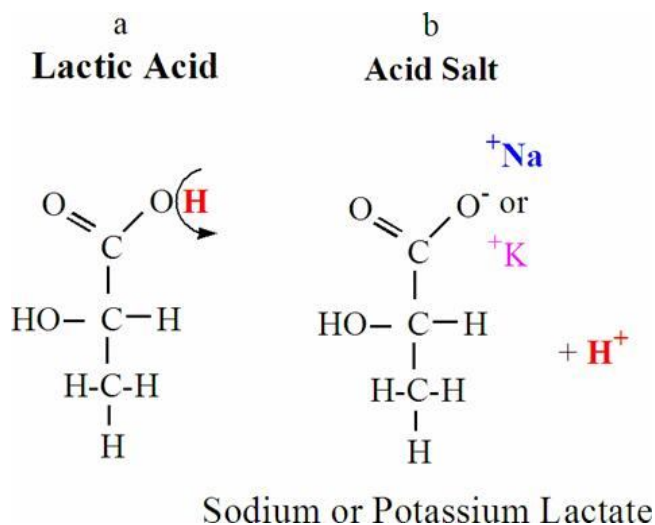
21 metabolites, 104 $L-M^+$ complexes, 17 reactions



Reaction	Enzyme	ΔH°
$HCrP + ADP + H^+ \leftrightarrow Cr + ATP$	Creatine kinase	+1
$ADP + ADP \leftrightarrow ATP + AMP$	Adenylate kinase	0
$AMP + H^+ \leftrightarrow IMP + NH_4$	AMP deaminase	+1
$ATP + H_2O \leftrightarrow ADP + Pi + H^+$	ATPase	-1
$Glycogen(n) + HPi \leftrightarrow Glycogen(n-1) + G1P$	Phosphorylase	0
$G1P \leftrightarrow G6P$	Phosphogluco mutase	0
$Glucose + ATP \leftrightarrow G6P + ADP + H^+$	Hexokinase	-1
$G6P \leftrightarrow F6P$	Glucose-6-phosphate isomerase	0
$F6P + ATP \leftrightarrow F1,6P + ADP + H^+$	Phosphofructokinase	-1
$F1,6P \leftrightarrow DHP + G3P$	Aldolase	0
$DHP \leftrightarrow G3P$	Phosphofructokinase	0
$G3P + HPi + NAD^+ \leftrightarrow 1,3BPG + NADH + H^+$	Glyceraldehyde-3-phosphate dehydrogenase	-1
$1,3BPG + ADP \leftrightarrow 3PG + ATP$	Phosphoglycerate kinase	0
$3PG \leftrightarrow 2PG$	Phosphoglycerate mutase	0
$2PG + ADP \leftrightarrow PEP$	Enolase	0
$PEP + ADP + H^+ \leftrightarrow Pyr + ATP$	Pyruvate kinase	+1
$Pyr + NADH + H^+ \leftrightarrow La + NAD^+$	Lactate dehydrogenase	+1



Association and Dissociation Constants



$$\text{Association constant} = K_a = \frac{[\text{HA}]}{[\text{H}^+][\text{A}^-]}$$

$$\begin{aligned}
 -\log K_a &= -\log \left(\frac{[\text{HA}]}{[\text{H}^+][\text{A}^-]} \right); \text{ for lactic acid with a } K_a = 2.13796 \times 10^{-4} \\
 pK_a &= -\log (2.13796 \times 10^{-4}) = -\log 0.000213796 = -(-3.67) = 3.67
 \end{aligned}$$

$$\text{Dissociation constant} = K_a = \frac{[H^+][A^-]}{[HA]}$$

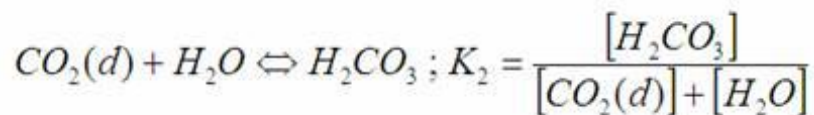
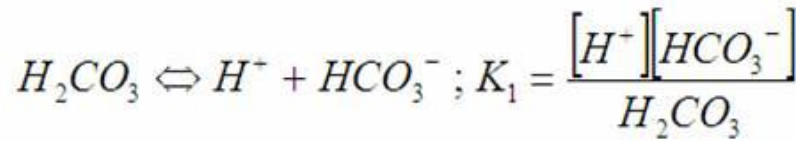
$$K_a (\text{lactic acid}) = \frac{[La^-] \times [H^+]}{[LaH]} = 4677.3514; \text{ where } \log_{10} 4677.3514 = 3.67$$

$$\log_{10} K_a (\text{lactic acid}) = 3.67$$

$$\text{when } [A^-] = [AH]; \log_{10} \frac{[A^-]}{[AH]} = 0$$

$$\text{then } pH = pKa + 0 \text{ or } pKa = pH$$

$$pH = pKa + \log_{10} \frac{[A^-]}{[AH]}; \text{ where } pKa = pH - \log_{10} \frac{[A^-]}{[AH]}$$

The dissociation constants for almost all metabolites in biological systems have been researched and compiled in a data base – NIST database.

*See NIST data base
See Excel spreadsheet*



Analytical Chemistry

$$K_H = \frac{[HL^{1-n}]}{[H^+][L^{n-}]} \quad K_{AH} = \frac{[AHL^{1+a-n}]}{[A^{a+}][H^+][L^{n-}]} \quad K_{AAH} = \frac{[A_2HL^{1+a-n}]}{[A^{a+}]^2[H^+][L^{n-}]}$$

$$L_{tot} = [L^{n-}] + K_H [H^+][L^{n-}] + K_{Hn} [H^+]^n [L^{n-}] + K_A [A^{a+}][L^{n-}] + K_{AH} [A^{a+}][H^+][L^{n-}] + \dots$$

$$\alpha_{-n} = \frac{[L^{n-}]}{L_{tot}} = \frac{1}{1 + K_H [H^+] + \dots + K_{Hn} [H^+]^n + K_A [A^{a+}] + K_{AH} [A^{a+}][H^+] + \dots}$$

$$[L^{n-}] = \alpha_{-n} L_{tot}$$

$$K_A [A^{a+}][L^{n-}] = [AL^{a-n}]$$



Amino Acids

		Second letter of codon			
		U	C	A	G
U	UUU	Phe	UCU Ser	UAU Tyr	UGU Cys
	UUC	Phe	UCC Ser	UAC Tyr	UGC Cys
	UUA	Leu	UCA Ser	UAA Stop	UGA Stop
	UUG	Leu	UCG Ser	UAG Stop	UGG Trp
C	CUU	Leu	CCU Pro	CAU His	CGU Arg
	CUC	Leu	CCC Pro	CAC His	CGC Arg
	CUA	Leu	CCA Pro	CAA Gln	CGA Arg
	CUG	Leu	CCG Pro	CAG Gln	CGG Arg
A	AUU	Ile	ACU Thr	AAU Asn	AGU Ser
	AUC	Ile	ACC Thr	AAC Asn	AGC Ser
	AUA	Ile	ACA Thr	AAA Lys	AGA Arg
	AUG	Met	ACG Thr	AAG Lys	AGG Arg
G	GUU	Val	GCU Ala	GAU Asp	GGU Gly
	GUC	Val	GCC Ala	GAC Asp	GGC Gly
	GUU	Val	GCA Ala	GAA Glu	GGA Gly
	GUG	Val	GCG Ala	GAG Glu	GGG Gly

Phenylalanine	Serine	Tyrosine	Cysteine
Leucine	Proline	Histidine	Tryptophan
Isoleucine	Threonine	Glutamine	Arginine
Methionine	Alanine	Asparagine	Serine
Valine		Lysine	Glycine
		Aspartate	
		Glutamate	



