Handout 1

Macroscopic thermodynamics

$$dU = \delta Q + \delta W$$

$$W = -\int P dV$$

$$\Delta S = \int \frac{\delta Q_{rev}}{T}$$

$\Delta S \geq 0$ for any spontaneous process in an *isolated* system

$\Delta G \leq 0$ for any spontaneous process in a system *at constant T and P*

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

$$C_V \equiv \left(\frac{dU}{dT}\right)_V = T\left(\frac{dS}{dT}\right)_V \qquad C_P \equiv \left(\frac{dH}{dT}\right)_P = T\left(\frac{dS}{dT}\right)_P$$

$$\Delta G(T) = \Delta H_0\left(1 - \frac{T}{T_0}\right) + \Delta C_p\left[T - T_0 - T\ln\left(\frac{T}{T_0}\right)\right] \qquad \text{for constant } C_P$$

Microscopic thermodynamics

$$S(state) = k_B \ln \Omega\,(state)$$

$$\wp(config) \propto e^{-\frac{U(config)}{k_B T}}$$

$$\wp(state) \propto e^{-\frac{G(state)}{k_B T}} \qquad \text{at constant } T, P$$

Reaction kinetics

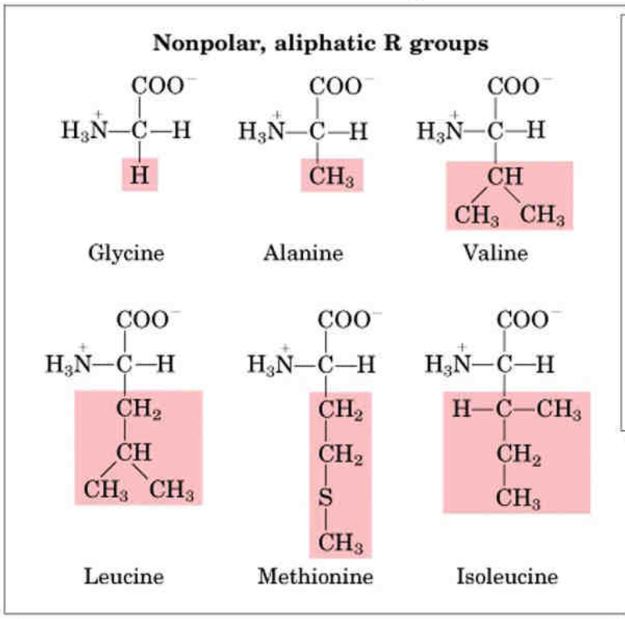
$$A \leftrightarrow B$$

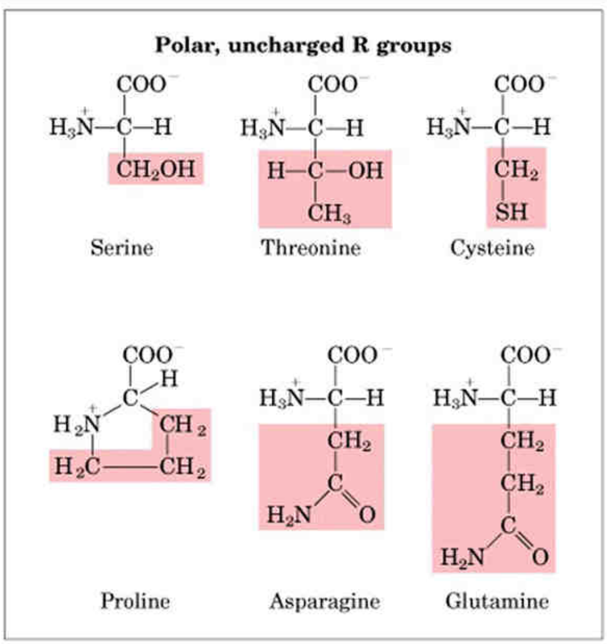
$$\text{reaction rate} = -\frac{d[A]}{dt} = \frac{d[B]}{dt} = k_f[A] - k_r[B]$$

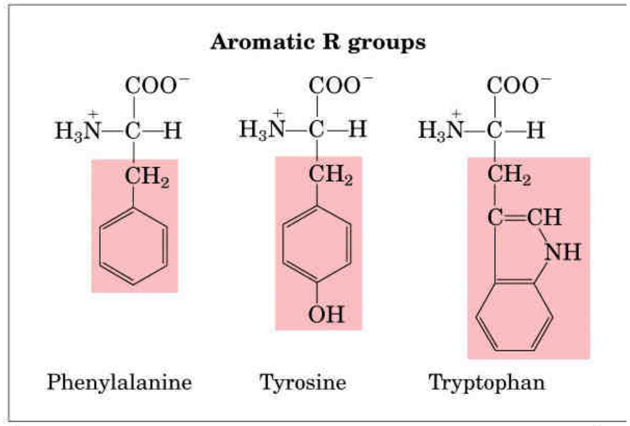
$$k_f = k_{f,0}e^{-\frac{\Delta G^{\ddagger}}{RT}}$$

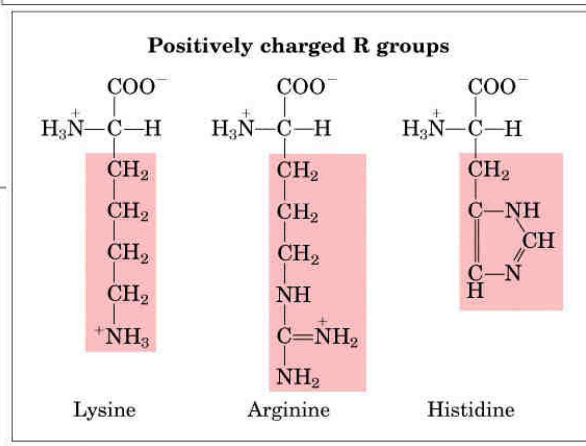
$$K_{eq} \equiv \exp\left(-\frac{\Delta G^{\circ}_{rxn}}{RT}\right) = \frac{[B]}{[A]} = \frac{k_f}{k_r}$$

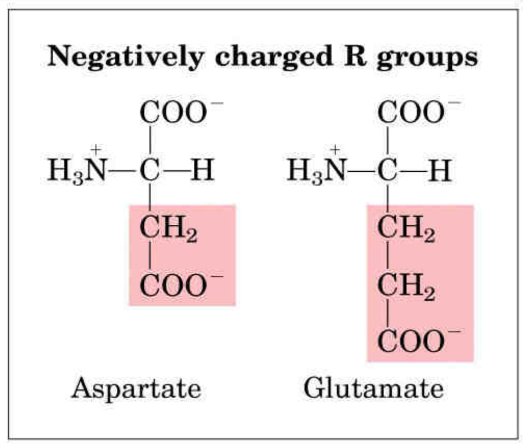
Twenty standard Amino Acids











alanine	ALA	A	isoleucine	ILE	I	arginine	ARG	R
cysteine	CYS	C	lysine	LYS	K	serine	SER	S
aspartic acid	ASP	D	leucine	LEU	L	threonine	THR	T
glutamic acid	GLU	E	methionine	MET	M	valine	VAL	V
phenylalanine	PHE	F	asparagine	ASN	N	tryptophan	TRP	W
glycine	GLY	G	proline	PRO	P	tyrosine	TYR	Y
histidine	HIS	H	glutamine	GLN	Q			