Bioelectronics

Waseda University
Graduate school of information, production and systems,
Production system

Professor.
Takeo Miyake

Schedule

[Fundamentals]

1. 4/15 Basic chemical and biochemical concepts
2. 4/22 Basic biophysical concepts
3. 4/29 Basic bioelectrochemical concepts1
4. 5/13 Basic bioelectrochemical concepts2

[Applications]

5. 5/20 Cancel (Homework1 and 2)
6. 5/27 Biosensors and bioelectronics1
7. 6/03 Cancel (Homework3 and 4)
8. 6/10 Student seminar
9. 6/17 Biosensors and bioelectronics2
10. 6/24 From bioelectronics (electron) to iontronics (ion)1
11. 7/01 From bioelectronics (electron) to iontronics (ion)2
12. 7/ 8 Wearable applications1
13. 7/15 Wearable applications2
14. 7/22 Student seminar

ワセぽち

https://my.waseda.jp/a

Key:

Q: I can understand in

A1: English
A2: Japanese
A3: Both
A4: Neither

ワセぽち

https://my.waseda.jp/a

Key:

Q: What is your major (or background)?

A1: Mathematics
A2: Computer science
A3: Physics
A4: Chemistry
A5: Electronics
A6: Biology
A7: Mechanics
A8: The others

ワセぽち

https://my.waseda.jp/a

Key:

Q: How understanding of "bioelectronics" before today's class?

A1: Extremely knowing
A2: Very knowing
A3: Somewhat knowing
A4: Mostly unknowing
A5: Totally unknowing

Evaluation

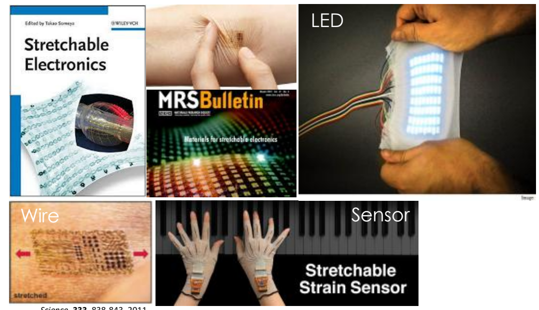
No examination

Reports: ca. 70%
(Presentation?)

Class participation
(Attendance):
ca. 30%

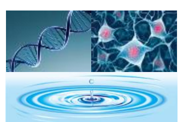
TIME Photo-Illustration (Sept 2014)

Wearable devices



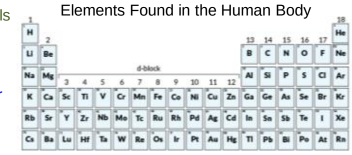
Science, **333**, 838-843, 2011

Interfacial Mismatch

Conventional Electronics		Human body
	Recording Biotransducer Stimulating	
Hard		**Soft**
Electron/Hole		**Ion control**
Dry		**Wet**

The elements in human body

Elements Found in the Human Body



How many elements did we find in the human body?

Which element is the most abundant in the human body by weight?

Homework1

体内に存在する元素を３つ選び、体内でどのように働いているかを示し，その説明をまとめよ（図があると望ましい）．

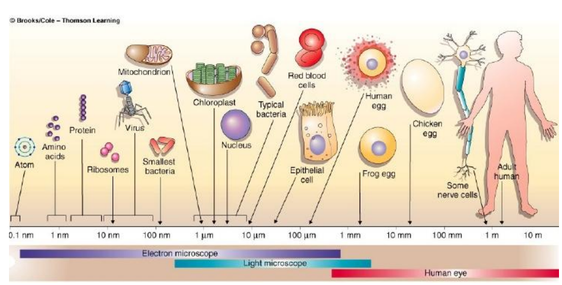
Choose three elements in our body, and the summarize as the following contents (any pages, including the figures and references).

1. The chosen three elements（選んだ3元素は何か？）
2. Why the elements are important in our body? （なぜ重要？）
3. How the elements work in our body?（どう働く？）
4. Conclusions and future perspective（結論と将来性）
5. Reference or book（参考文献、号、巻、ページ）

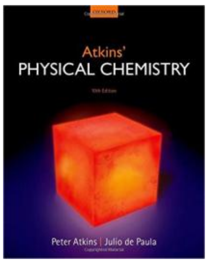
Deadline: Apri 27 2025

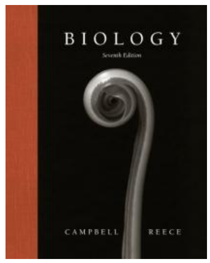
✓ Upload electrical file (MS word or pdf)to this lecture in MyWaseda

Biological size and cell diversity



Basic chemical and biochemical concepts





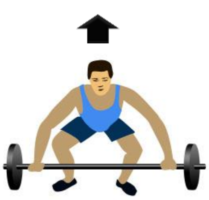
Bioenergy

+

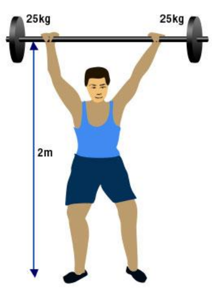
Work for lifting

Energy

Kinetic energy



Potential energy



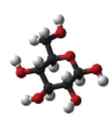
Bioenergy

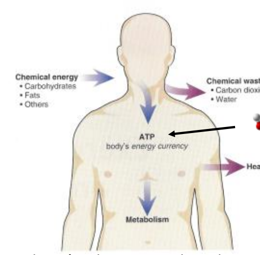
Kinetic energy

Potential energy

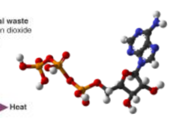
<u>Motion of molecules</u>

Glucose





ATP



mechanical energy, heat energy

Bioenergy

$\boxed{\mu_i=}$

Potential energy

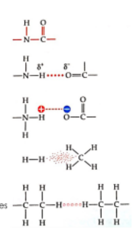
<u>Chemical bond</u>

<u>Chemical potential: μ</u>

ΔG: the Gibbs energy change

n_i: the number of moles of each substance

Covalent bond	Sharing of electron pairs 2.17-4.77 eV (209-460 kJ/mol)	
Hydrogen bond	Sharing of H atom 0.13-0.30 eV (12.5-29.3 kJ/mol)	
Ionic interaction	Attraction of opposite charges 0.13-0.30 eV (12.5-29.3 kJ/mol)	
Van der Waals interaction	Interaction of electron clouds 0.043 eV (4.184 kJ/mol)	
Hydrophobic interaction	Interaction of nonpolar substrates 0.043-0.086 eV (4.184-8.368 kJ/mol)	



Bioenergy

$\boxed{\mu_i=}$

Potential energy

<u>Chemical bond</u>

<u>Chemical potential: μ</u>

ΔG: the Gibbs energy change

n_i: the number of moles of each substance

The Gibbs energy (change: ΔG)

<u>*$\Delta G = \Delta H - T\Delta S$ (at constant T)*</u>

H: The enthalpy

T: Temperature

S: The Entropy

1st Law Thermodynamics

Energy conservation in a closed system

$\Delta E_{universe} = \Delta E_{sys} + \Delta E_{surrounding} = 0$

$\Delta E = q + w$

Change internal energy | Hear transfer | Work done by/on system

E = sum kinetic energy/motion of molecules, and potential

The internal energy U:

$\Delta U = q + w$

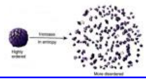
The enthalpy $H = U+pV$:

$\Delta H = \Delta U + \Delta(pV)$
$= \Delta U + p\Delta V$ (at constant P)

2nd Law Thermodynamics

Isolated system = Entropy change of universe always increase

$\Delta S_{universe} = \Delta S_{sys} + \Delta S_{surrounding} > 0$

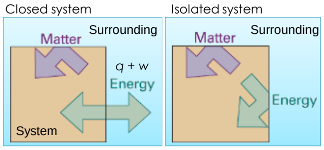


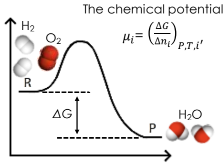
The Gibbs energy (change: ΔG)

$\Delta G = \Delta H - T\Delta S$ (at constant T)

The chemical potential

$\mu_i = \left(\frac{\partial G}{\partial n_i}\right)_{P,T,i'}$





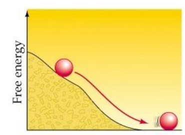
The Gibbs free energy

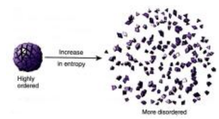
$G = H-TS$ (= $U+PV-TS$)

Change in Gibbs energy (ΔG) at constant T

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

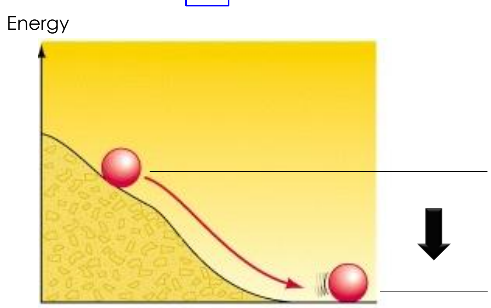
Spontaneous reaction: $-\Delta G$





The Gibbs free energy

$\Delta G = \boxed{\Delta H} - T\Delta S$



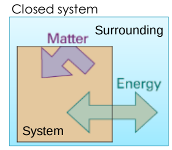
The 1st law of thermodynamics

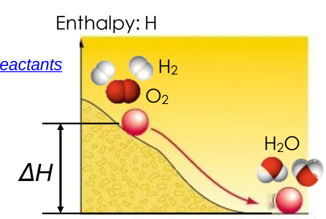
Energy conservation in a closed system

Change in energy in system = energy in – energy out

(Ex.) Enthalpy: H

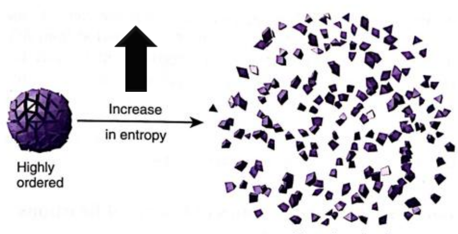
$\Delta H = H_{products} - H_{reactants}$





The Gibbs free energy

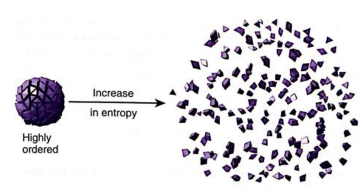
$\Delta G = \Delta H - T\boxed{\Delta S}$



The 2nd law of thermodynamics

The entropy of an isolated system tends to increase.

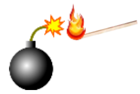
$\Delta S_{univ} = \Delta S_{system} + \Delta S_{surroundings} > 0$

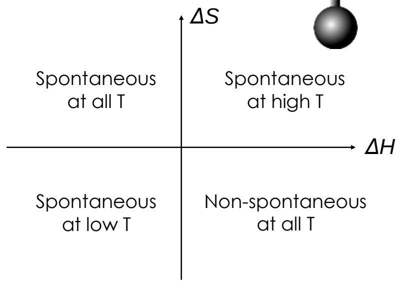


The Gibbs free energy

Spontaneous reaction: - ΔG

$$\Delta G = \Delta H - \boxed{T}\Delta S$$





The Gibbs free energy

$G = H\text{-}TS = U\text{+}PV\text{-}TS$

Change in Gibbs energy (ΔG) at constant T

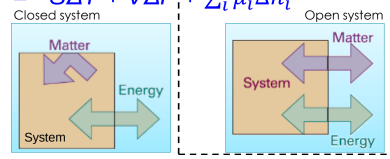
$\Delta G(n, P, T) = \Delta U + V\Delta P + P\Delta V - S\Delta T - T\Delta S$

$= (\Delta U + P\Delta V - T\Delta S) - S\Delta T + V\Delta P$

$\Delta U = T\Delta S - P\Delta V$

$= - S\Delta T + V\Delta P + (\mu_A \Delta n_A + \mu_B \Delta n_B +)$

$= - S\Delta T + V\Delta P + \sum_i \mu_i \Delta n_i$



The Chemical potential

$\Delta G(n, P, T) = - S\Delta T + V\Delta P + \sum_i \mu_i \Delta n_i$

P and T, Constant

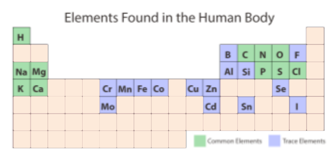
$\Delta G = \sum_i \mu_i \Delta n_i \longrightarrow \boxed{\mu_i = \left(\frac{\Delta G}{\Delta n_i}\right)_{P,T,i}}$

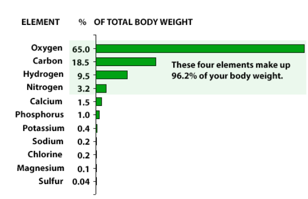
$\Delta G = \quad = \sum_i \mu_i \Delta n_i$

Chemical potential in the liquid

$$\mu_i(l) = \mu_i^{\phi, ideal} + RT\ln a_i$$

The elements of human body





Chemical bonds and interaction

Covalent bond	Sharing of electron pairs 2.17-4.77 eV (209-460 kJ/mol)	
Hydrogen bond	Sharing of H atom 0.13-0.30 eV (12.5-29.3 kJ/mol)	
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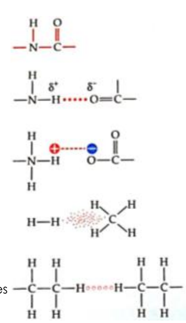
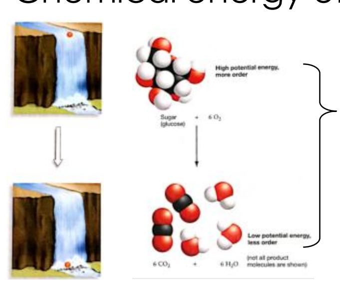


Chemical energy of Glucose



How much (ΔG)?

Table 4.2 Standard Gibbs energies of formation at 298.15 K*

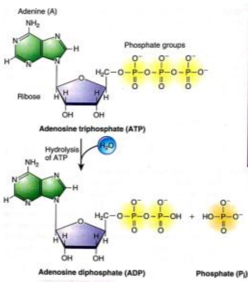
Substance	$\Delta_f G^{\circ}$/(kJ mol^{-1})
Gases	
Carbon dioxide, CO_2	−394.36
Methane, CH_4	−50.72
Nitrogen oxide, NO	+86.55
Water, H_2O	−228.57
Liquids	
Ethanol, CH_3CH_2OH	−174.78
Hydrogen peroxide, H_2O_2	−120.35
Water, H_2O	−237.13
Solids	
α-D-Glucose $C_6H_{12}O_6$	−917.2
Glycine, $CH_2(NH_2)COOH$	−532.9
Sucrose, $C_{12}H_{22}O_{11}$	−1543
Urea, $CO(NH_2)_2$	−197.33
Solutes in aqueous solution	
Carbon dioxide, CO_2	−385.98
Carbonic acid, H_2CO_3	−623.08
Phosphoric acid, H_3PO_4	−1018.7

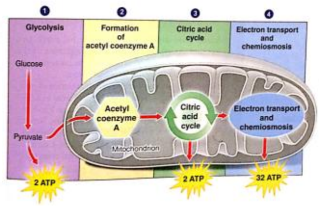
*Additional values are given in the Data section.

$C_6H_{12}O_6(s) + 6O_2(g) \rightarrow 6CO_2(g) + 6H_2O(l)$

ΔG = - _____ kJ/mol, $\Delta E = \Delta G/\text{-}nF$ = _____ V

Why ATP



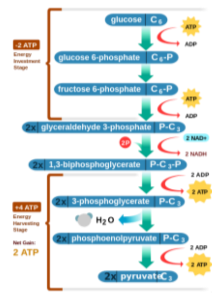


$ATP^{4-}(aq) + H_2O(l) \rightarrow$
$ADP^{2-}(aq) + P_i^{2-}(aq)$

ΔG = -32 kJ/mol, ΔE = ΔG/-nF = 0.33 V

Use ATP to drive endergonic reactions

① Glycolysis



$Glucose(s) + phosphate^{2-}(aq) \rightarrow$
$Glucose\text{-}6\text{-}phosphate^{2-}(aq) + H_2O\ (aq)$

Endergonic: *ΔG = kJ/mol, ΔE = V*

$ATP^{4-}(aq) + H_2O(l) \rightarrow ADP^{2-}(aq) + P_i^{2-}(aq)$

Exergonic: ΔG = kJ/mol, ΔE = V

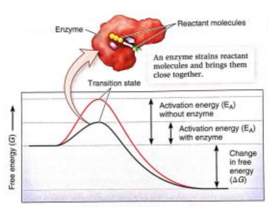
Coupled reaction:

$Glucose(s) + ATP^{4-}(aq) \rightarrow$
$Glucose\text{-}6\text{-}phosphate^{2-}(aq) + ADP^{2-}(aq)$

Exergonic: ΔG = kJ/mol, ΔE = V

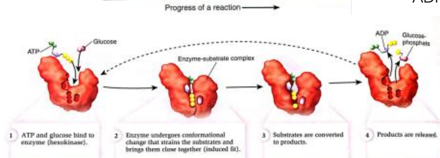
Enzyme increase the rates of reactions

Glucose
ATP



ΔG = -18.2 kJ/mol

Glucose-6P
ADP



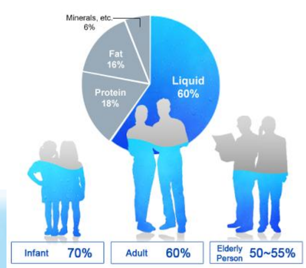
Water properties

High melting and boiling point
(Specific heat)

Latent heat of vaporization

Solubility

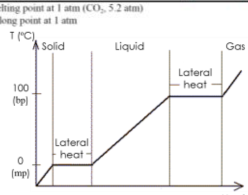
Polarity, hydrogen bond,
hydrophobic interaction

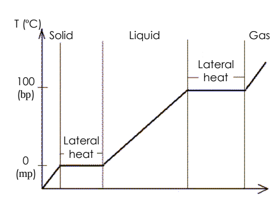


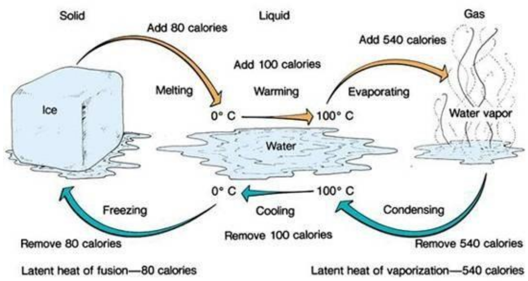
Melting and boiling points of various samll molecules

molecules		molar mass (g/mol)	mp (˚C)	bp (˚C)
CH_4	methane	16	-183	-162
H_2O	water	18	0	100
N_2	nitrogen	24	-210	-196
O_2	oxygen	32	-219	-183
O_3	ozone	48	-197	-112
CO_2	carbon dioxide	44	-57	-79

mp: melting point at 1 atm (CO_2, 5.2 atm)
bp: boilong point at 1 atm







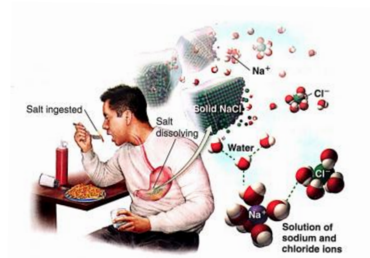


Figure 2.16 NaCl crystals dissolving in water. The ability of water to dissolve sodium chloride crystals depends on the electrical attraction between the polar water molecules and the charged sodium and chloride ions. Water molecules surround each ion as it becomes dissolved.

$NaCl(s) \rightarrow Na^+(aq) + Cl^-(aq)$ (0.09eV (-9 kJ/mol))

Ionic bond: Na^+Cl^-

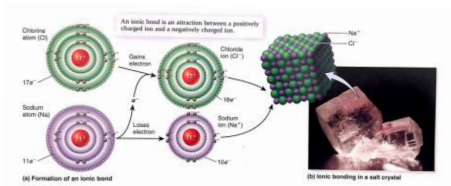
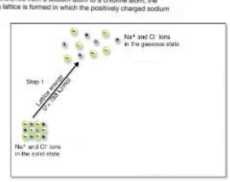


Figure 2.12 Ionic bonding in table salt (NaCl).

$Na^+(g) + Cl^-(g)$

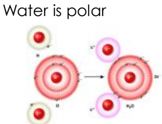
ΔH_{LE} = 788 KJ/mol = 8.1 eV

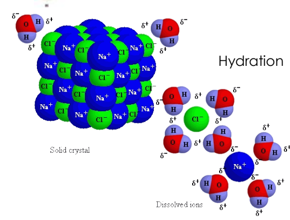
NaCl(s)

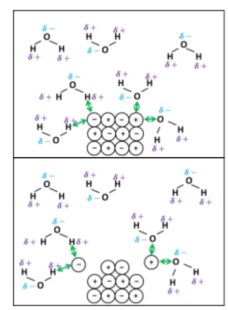


Water and NaCl interaction

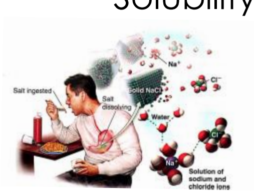
- Water is polar







Solubility of water



ΔG = ΔH - TΔS

$Na^+(g) + Cl^-(g)$

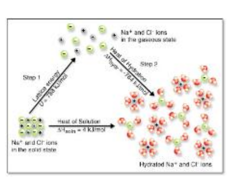
Na(g) + Cl(g)

ΔH_{LE} = 788 KJ/mol

ΔH_{hyd} = 784 KJ/mol

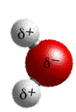
$Na^+(aq) + Cl^-(aq)$

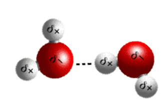
NaCl(s)+aq ΔH_{sol} = 4 KJ/mol

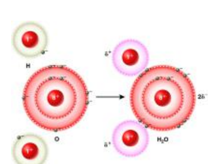


Properties of water

- Water is polar
- Hydrogen bonds between water molecules







Weak bond (20 kJ/mol)

Chemical bond of O-H (460 kJ/mol)

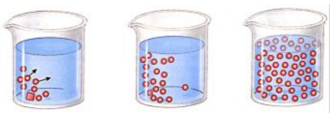
Ionic mobilities

Synoptic table 21.6* Ionic mobilities in water at 298 K

	$u/(10^{-8}\ m^2\ s^{-1}\ V^{-1})$		$u/(10^{-8}\ m^2\ s^{-1}\ V^{-1})$
H^+	36.23	OH^-	20.64
Na^+	5.19	Cl^-	7.91
K^+	7.62	Br^-	8.09
Zn^{2+}	5.47	SO_4^{2-}	8.29

Diffusion model (Einstein-Stokes equation)

$$\boxed{\mu_i = \frac{Dq}{k_B T}}$$



Ionic mobilities

Synoptic table 21.6* Ionic mobilities in water at 298 K

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Diffusion model (Einstein-Stokes equation)

$$\boxed{\mu_i = \frac{Dq}{k_B T}}$$

TABLE 1.6 Conductivity and Diffusion Coefficients of Selected Ions at Infinite Dilution in Water at 25°C

Cation	$\lvert z \rvert$	λ, $S \cdot cm^2 \cdot mol^{-1}$	$D \times 10^5$, $cm^2 \cdot s^{-1}$	Anion	$\lvert z \rvert$	λ, $S \cdot cm^2 \cdot mol^{-1}$	$D \times 10^5$, $cm^2 \cdot s^{-1}$
H^+	1	349.8	9.30	OH^-	1	197.6	5.25
Li^+	1	38.7	1.03	F^-	1	55.4	1.47
Na^+	1	50.1	1.33	Cl^-	1	76.3	2.03
K^+	1	73.5	1.95	NO_3^-	1	71.4	1.90
Ca^{2+}	2	119.0	0.79	ClO_4^-	1	67.3	1.79
Cu^{2+}	2	107.2	0.71	SO_4^{2-}	2	160.0	1.06
Zn^{2+}	2	105.6	0.70	CO_3^{2-}	2	138.6	0.92
O_2	—	—	2.26	HSO_4^-	1	50.0	1.33
H_2O	—	—	2.44	HCO_3^{-1}	1	41.5	1.11

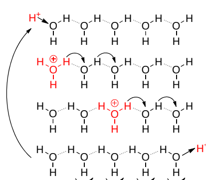
Ionic mobilities

Synoptic table 21.6* Ionic mobilities in water at 298 K

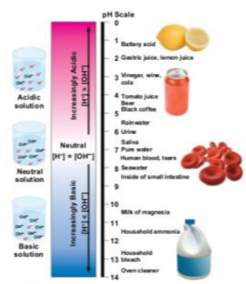
	$u/(10^{-8}\ m^2\ s^{-1}\ V^{-1})$		$u/(10^{-8}\ m^2\ s^{-1}\ V^{-1})$
H^+	36.23	OH^-	20.64
Na^+	5.19	Cl^-	7.91
K^+	7.62	Br^-	8.09
Zn^{2+}	5.47	SO_4^{2-}	8.29

Grotthuss mechanism

$$\boxed{\mu_H \propto \frac{1}{T} exp\left(\frac{-E_A}{K_B T}\right)}$$



pH, H^+ and OH^-



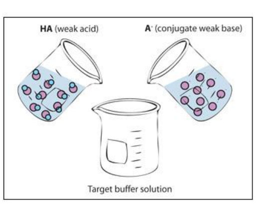
$$pH + pOH = 14$$

$$pH = -log_{10} a_{H^+} = log_{10}\frac{1}{a_{H^+}}$$

$$E = E^0 + \frac{RT}{F} ln(a_{H^+})$$
$$= E^0 - \frac{2.303RT}{F} pH$$

$$pOH = -log_{10} a_{OH^-} = log_{10}\frac{1}{a_{OH^-}}$$

Buffer solution –constant pH-



Henderson-Hasselbalch equation

$$pH = pK_a + log_{10}\left(\frac{[A^-]}{[HA]}\right)$$

Ex. Phosphate buffer (0.1M, pH7.4)

$H_2PO_4^- \leftrightarrows H^+ + HPO_4^{2-}$

$$pH = pK_a + log_{10}\left(\frac{[HPO_4{}^{2-}]}{[H_2PO_4{}^-]}\right)$$

Acid dissociation: 7.21

$$7.4 = 7.21 + log_{10}\left(\frac{[HPO_4{}^{2-}]}{[H_2PO_4{}^-]}\right) \quad (1)$$

$$0.1 = [H_2PO_4{}^-] + [HPO_4{}^{2-}] \quad (2)$$

$H_2PO_4{}^- = 0.0392\ M$

$HPO_4{}^{2-} = 0.0608\ M$