INTERNATIONAL COLLEGE OF PHARMACEUTICAL INNOVATION
国际创新药学院

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|---|---|
| **Class** | Pharm, BioPharm |
| **Course** | Fundamentals of Medicinal & Pharmaceutical Chemistry |
| **Code** | FUNCHEM.5 |
| **Title** | Chemical Equations and Reactions. Composition of Physiological Solutions |
| **Lecturer** | Prof. Xinchen Teng |
| **Date** | 2024-10-16 |

# RECOMMENDED READING

- General Chemistry - The Essential Concepts by Chang and Goldsby (7$^{th}$ edition)
  - Section 2.2 - The structure of atom
  - Section 2.5 - Molecules and Ions
  - Section 2.6 - Chemical Formulas
  - Section 3.1 - Atomic mass
  - Section 3.2 - Avogadro's Number and the Molar Mass
  - Section 3.3 - Molecular Mass
  - Section 3.7 - Chemical Reactions and Chemical Equations
  - Section 4.1 - General Properties of Aqueous Solutions
  - Section 4.5 - Concentration of Solutions

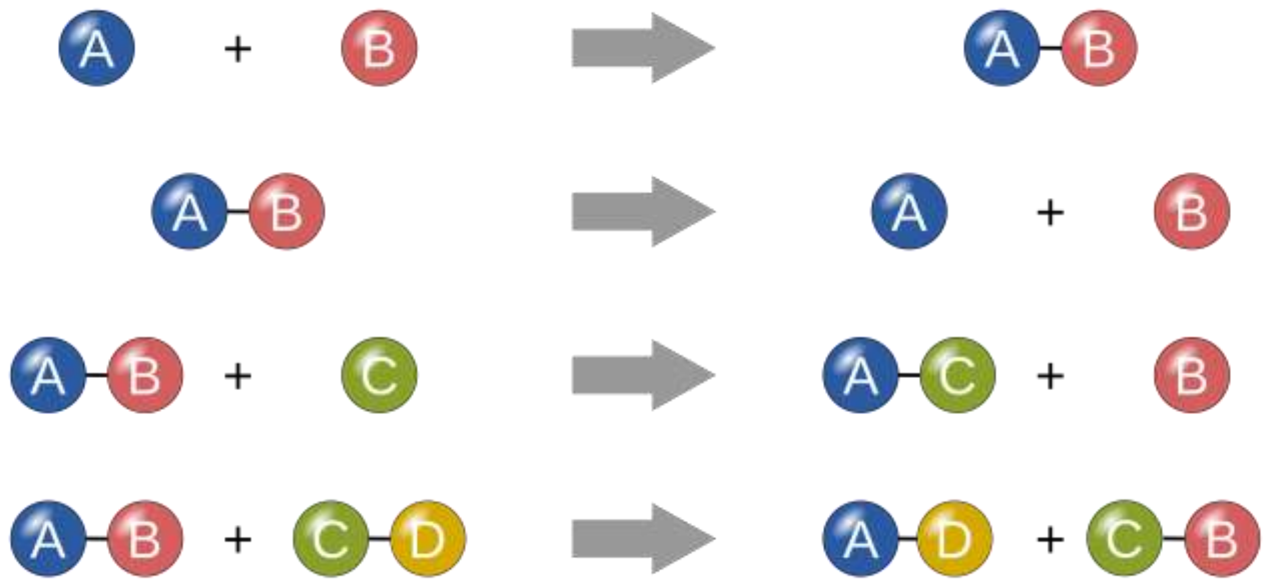
# FUNCHEM.5 Learning Outcomes

- Define ‘molecule’, molecular formula’, ‘molecular mass’, ‘mole’, ‘Avogadro’s number’.
- Solve calculations involving moles.
- Demonstrate method of balancing chemical equations.
- Define ‘solution’ and relate human body to solutions in terms of blood plasma, extra- and intracellular body fluids.
- Apply medical applications to solutions.
- Define ‘isotonic’, ‘hypertonic’ and ‘hypotonic’ solutions in relation to red blood cells and be able to explain the effect of placing red blood cells in each of these solutions.
- Recall and calculate percentage solutions (w/v %, w/w %, mg %), parts per million (ppm) and molar (M) concentrations.

# Chemical Reactions

A process in which a substance ( or substances) is changed into one or more new substances.

A chemical equation uses chemical symbols to show what happens during a chemical reaction



# Chemical Equations

REACTANTS

PRODUCTS

$$6CO_{2(g)} + 6H_2O_{(l)} \xrightarrow{\text{sunlight}} \underset{\text{Glucose}}{C_6H_{12}O_{6(s)}} + 6O_{2\,(g)}$$

Prefix numbers refer to the whole molecule

Subscript numbers refer to previous atom only

Symbols (s), (l) and (g) indicate the state of the product or reactant (aq) = dissolved in water

# ‘Recipe’ to make glucose

$$CO_2 + H_2O \xrightarrow{\text{sunlight}} \underset{\text{Glucose}}{C_6H_{12}O_6} + O_2$$

<u>Balanced</u>

$$6CO_2 + 6H_2O \xrightarrow{\text{sunlight}} \underset{\text{Glucose}}{C_6H_{12}O_6} + 6O_2$$

## How do we measure quantities?

$$6CO_2 + 6H_2O \xrightarrow{\text{sunlight}} C_6H_{12}O_6 + 6O_2$$

Glucose

6 molecules of $CO_2$ weighs $4.78 \times 10^{-22}$g

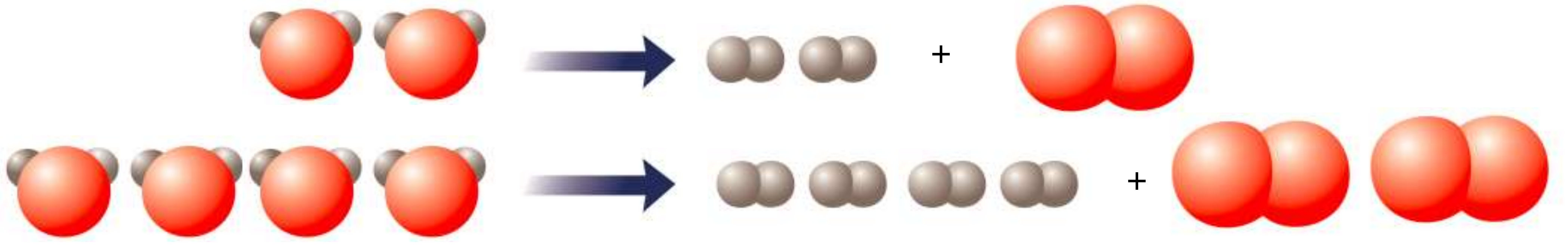

on the balance 0.000000000000000000000478 g

We need to relate mass of a substance to the number of atoms/molecules present

# Equations On a Macroscopic Scale

- Instead of thinking atoms or molecules, scale up everything to moles

$$2H_2O(l) \xrightarrow{\text{electricity}} 2H_2(g) + O_2(g)$$



- Chemical equations can be multiplied by any number as long as both sides are multiplied by the same number

$$(2 \times 6.022 \times 10^{23})H_2O(l) \xrightarrow{\text{electricity}} (2 \times 6.022 \times 10^{23})H_2(g) + (6.022 \times 10^{23})O_2(g)$$

$$2 \text{ mol } H_2O(l) \xrightarrow{\text{electricity}} 2 \text{ mol } H_2(g) + 1 \text{ mol } O_2(g)$$

# Molar Mass

Molar mass is the mass in grams
of 1 mole of molecules or 1 mole of atoms

The unit for molar mass is g/mol

1 mole of atoms contains $6.022 \times 10^{23}$ atoms
and has a mass = atomic mass

1 mole of molecules contains $6.022 \times 10^{23}$
molecules and has a mass = molecular mass

# How To "Read" Chemical Equations

$$2\ Mg + O_2 \longrightarrow 2\ MgO$$

2 atoms Mg + 1 molecule $O_2$ makes 2 formula units MgO

2 moles Mg + 1 mole $O_2$ makes 2 moles MgO

48.6 grams Mg + 32.0 grams $O_2$ makes 80.6 g MgO

**NOT**

2 grams Mg + 1 gram $O_2$ makes 2 g MgO

# How To Write A Chemical Equation

- Identify **reactants** and **products** and write a word equation

$$\text{water} \longrightarrow \text{hydrogen gas} + \text{oxygen gas}$$

- Write symbols for elements (or formulas for elements existing as polyatomic molecules) and formulas for compounds

$$H_2O \longrightarrow H_2 + O_2$$

- Balance by changing coefficients in front of symbols and formulas. Simplify the coefficients if they have a common divisor.

$$2H_2O \longrightarrow 2H_2 + O_2$$

- Add symbols indicating phases of substances: (s) for a solid, (l) for a liquid, (g) for a gas and (aq) for a solution of a substance in water
- Add reaction condition over the arrow

$$2H_2O(l) \xrightarrow{\text{electricity}} 2H_2(g) + O_2(g)$$

# Balancing Equations

- Begin with the compound that has the most atoms or the most kinds of atoms and use one of these atoms as a starting point

$$CH_4O + O_2 \longrightarrow CO_2 + H_2O$$

- Balance elements that appear only once on each side of the arrow first

$$CH_4O + O_2 \longrightarrow CO_2 + 2H_2O$$

- Then balance elements that appear more than once on a side. Balance free elements last

$$CH_4O + 3/2O_2 \longrightarrow CO_2 + 2H_2O$$

- Clear fractions to make coefficients whole numbers

$$2CH_4O + 3O_2 \longrightarrow 2CO_2 + 4H_2O$$

- Add reaction condition and symbols indicating phases

$$2CH_4O(l) + 3O_2(g) \xrightarrow{\text{spark}} 2CO_2(g) + 4H_2O(l)$$

# Examples

$$C_2H_5OH_{(l)} + O_{2(g)} \longrightarrow H_2O_{(l)} + CO_{2\,(g)}$$

2C 6H 3O

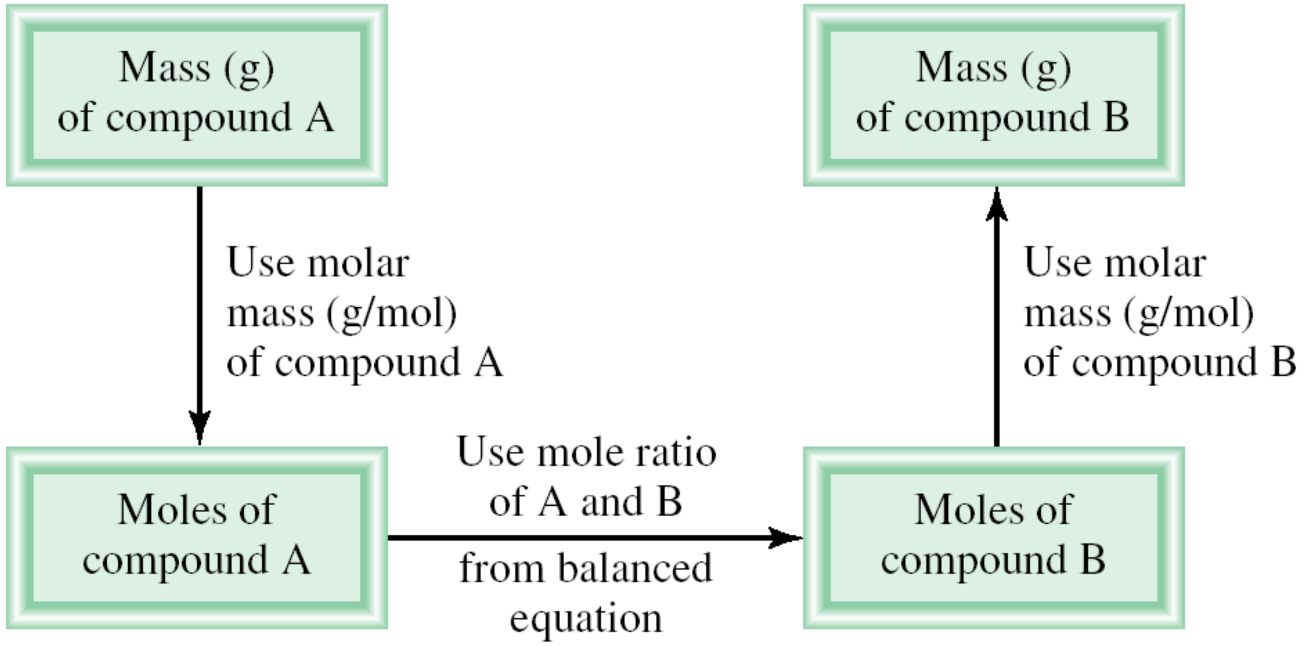
1 C 2H 3O

$$C_2H_5OH_{(l)} + 3\,O_{2(g)} \longrightarrow 3\,H_2O_{(l)} + 2\,CO_{2\,(g)}$$

2C 6H 7O

2C 6H 7O

# Calculate the Amounts of Reactants and Products



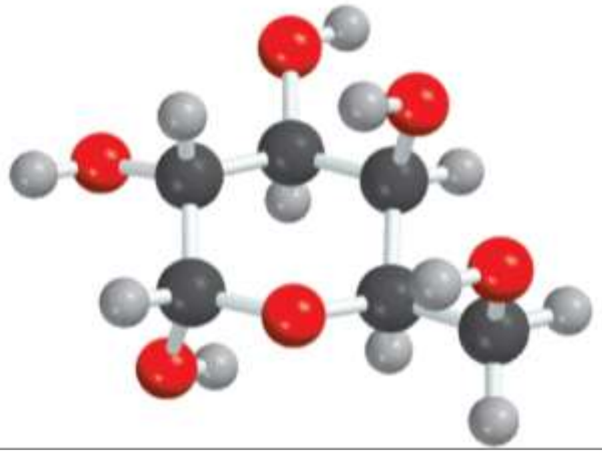

1. Write balanced chemical equation
2. Convert quantities of reactant A (in grams) into moles
3. Use the mole ratio in the balanced equation to calculate the number of moles of product B formed.
4. Convert moles of product to grams of product

## Example

A general overall equation for degradation of glucose ($C_6H_{12}O_6$) to carbon dioxide ($CO_2$) and water ($H_2O$):

$$C_6H_{12}O_6 + 6O_2 \longrightarrow 6CO_2 + 6H_2O$$

If 856 g of $C_6H_{12}O_6$ is consumed by a person over a certain period, what is the mass of $CO_2$ produced?



*$C_6H_{12}O_6$*

$$\textbf{No. of moles} = \frac{\textbf{mass (g)}}{\textbf{Molar mass (g/mol)}}$$

$$C_6H_{12}O_6 + 6O_2 \longrightarrow 6CO_2 + 6H_2O$$

mass $\qquad\qquad$ mass ??

moles $\longrightarrow$ moles

*Step 1:* The balanced equation is given in the problem.

*Step 2:* To convert grams of $C_6H_{12}O_6$ to moles of $C_6H_{12}O_6$

Moles = mass/ molar mass = 856/180.2 = 4.75 mol $C_6H_{12}O_6$

*Step 3:* From the mole ratio, we see that

1 mol $C_6H_{12}O_6$ : 6 mol $CO_2$

Therefore, the number of moles of $CO_2$ formed is

4.75 x 6 = 28.5 mol

$$C_6H_{12}O_6 + 6O_2 \longrightarrow 6CO_2 + 6H_2O$$

$$\begin{tikzcd}
\text{mass} \arrow[d] & \text{mass ??} \\
\text{moles} \arrow[r] & \text{moles} \arrow[u]
\end{tikzcd}$$

*Step 4:* Finally, the number of grams (mass) of $CO_2$ formed is given by:

Moles = mass/molar mass (rearrange)

Mass = moles x molar mass (of $CO_2$)

Mass = 28.5 x 44.01 = 1,254.3 g

# What is a solution

Solutions are homogeneous mixture of two or more substances, can be formed in any state of matter; that is they may be solid, liquid, or gas

| Solute | Solvent |
|---|---|
| Solid/ liquid/ gas | liquid/ gas<br>Present in larger amount |


Solute Solvent Saline solution

Solute – the substance being dissolved

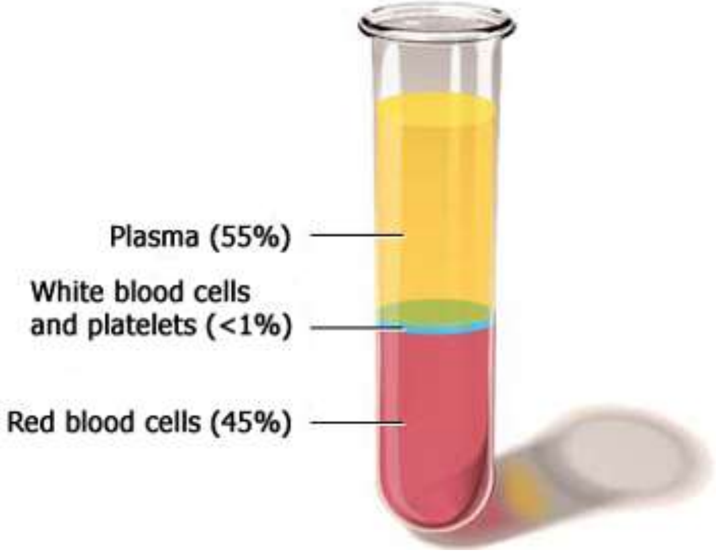
Solvent – the substance “doing” the dissolving

**The human body is made up of ~ 60% water..**

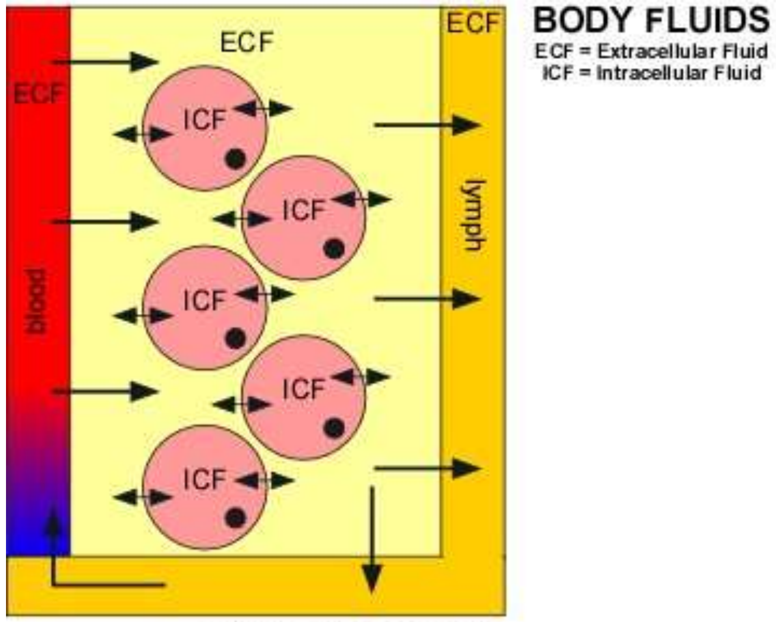
**….hence the body is a big solution**

Approximately 40 Litres

- 3 litres of blood plasma

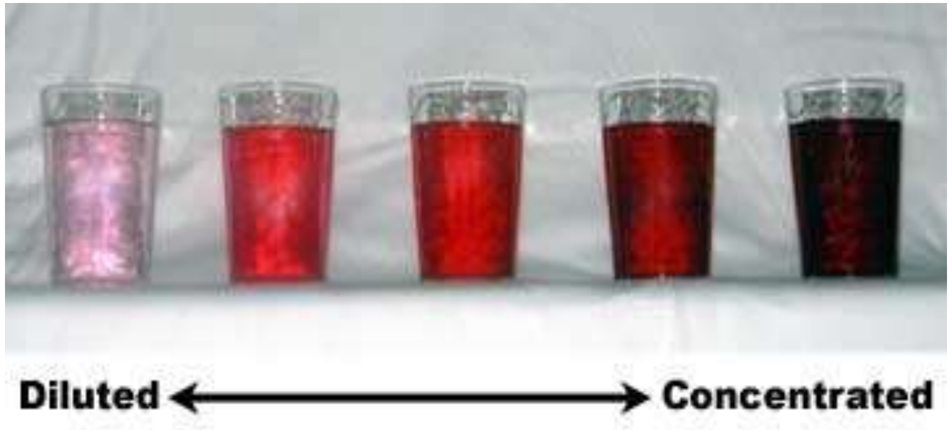



- 25 litres of intracellular fluid
- 12 litres of extracellular fluid



# Concentration of a Solution

The concentration of a solution is the amount of solute present in a given amount of solvent, or a given amount of solution.




A dilute solution contains relatively little solute in a large quantity of solution

A concentrated solution contains a relatively large amount of solute in a given quantity of solution

For the sake of accuracy sometimes we need to know exact concentrations

# Concentration Expressed As Percent

$$\text{Weight/Volume percent (w/v \%)} = \frac{\text{g Solute}}{\text{100 mL Solution}} \times 100$$

$$\text{Weight/Weight percent (w/w \%)} = \frac{\text{g Solute}}{\text{100 g Solution}} \times 100$$

$$\text{Volume/Volume percent (v/v \%)} = \frac{\text{mL Solute}}{\text{100 mL Solution}} \times 100$$

Percentage Concentrations are used in clinical reports, medicines, intravenous drips, and oral rehydration packs

# Make Liquid Solution with Solid Solute


(a) An amount of solute is weighed out on an analytical balance and then

(b) A portion of the solvent is added to the volumetric flask.

(c) The mixture is swirled until *all* of the solute is dissolved.

(d) Additional solvent is added up to the mark on the volumetric flask.

the bottom of the meniscus touches the graduation line

# Make Liquid Solution from Liquid

Make solution from a concentrated one


**(a) A volume ($V_s$) containing the desired moles of solute ($M_s$) is measured from a stock solution of known concentration.**

**(b) The measured volume of stock solution is transferred to a second volumetric flask.**

**(c) The measured volume in the second flask is then diluted with solvent up to the volumetric mark [$(V_s)(M_s) = (V_d)(M_d)$].**

# Intravenous Drip

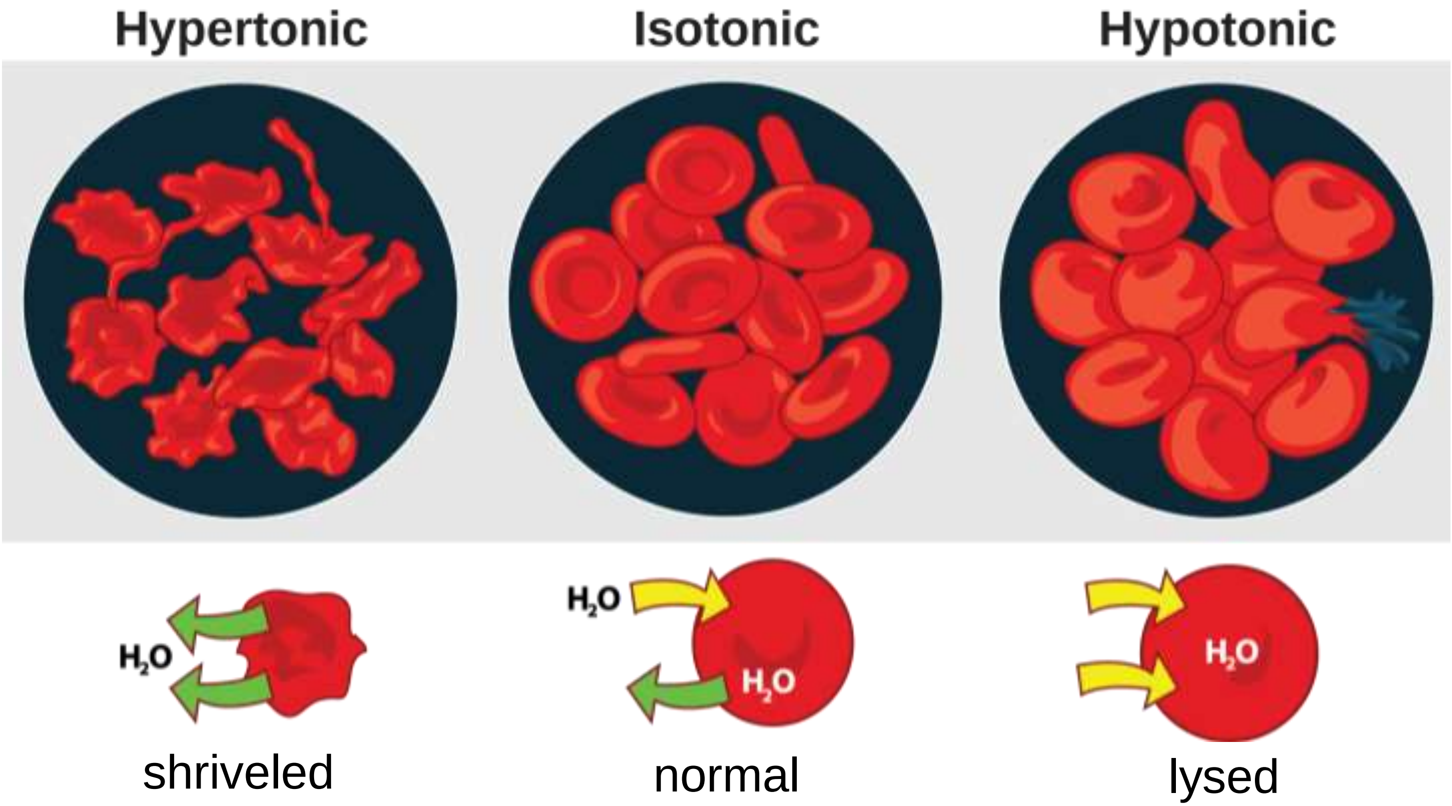
Intravenous (IV) therapy is the giving of substances directly into a vein


- Can’t Swallow safely (coma, under anaesthetic)
- Require medications which are destroyed by gastric juices or are poorly absorbed by the gastrointestinal tract
- Must rapidly increase the concentration of medication (e.g. morphine) or electrolyte
- Can’t drink enough to keep up with loss of fluids (major burns, severe diarrhoea, haemorrhage)

I.V. drip is usually isotonic with blood plasma

# Isotonic Solutions

For severe dehydration, if inject water directly, RBC will swell and burst (**Haemolysis**)




5% w/v glucose is nearly isotonic with blood plasma

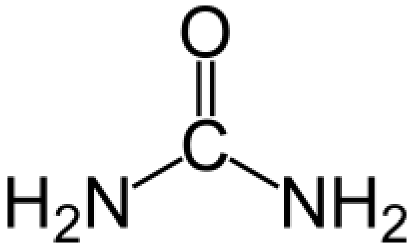
As the glucose is metabolised the water remains to rehydrate the body

# Concentration Expressed As Milligram Percent

$$\text{Milligram Percent (mg\%)} = \frac{\text{mg Solute}}{\text{100 mL Solution}} \times 100$$

*1 mg = 0.001 g

Blood Urea Nitrogen levels (BUN) level is measured in milligram percent (mg%)




Protein metabolised → Amino acids → Urea (kidneys)

↓

Urine

**Normal BUN = 7 – 21 mg BUN / 100 mL blood**

**= 7 - 21 mg%**

Elevated BUN level (azotemia) due to …..

- Impaired renal function
- Dehydration (lack of fluid volume to excrete waste products)
- Excessive protein intake or protein catabolism

An Infant suffering dehydration might have a BUN level of 32 mg%

i.e. 32 mg of urea per 100 mL of blood

or 0.032 g of urea in 100 mL of blood = 0.032 % w/v

# Concentration Expressed As Parts per Million

$$\text{Parts per Million (ppm)} = \frac{\text{mg Solute}}{\text{1 L Solution}}$$

Used to describe extremely dilute solutions
e.g. the concentration of toxic metals
present in drinking water

Some compounds are toxic to humans at 1 ppm!

# Molarity (*M*)

Molarity indicates the number of moles of a solute per liter of solution..

$$\boldsymbol{M} = \textbf{\textit{molarity}} = \frac{\text{Moles of solute}}{\text{Liters of solution}}$$

M (units, read as **molar**) = mol/L

# Make Solutions Of Given Molarity

How many grams of $KMnO_4$ (potassium permanganate) are needed to make 500.0 mL of $5.75 \times 10^{-4}$ M $KMnO_4$?

$$M = \frac{\text{amount of solute (mole)}}{\text{volume of solution (liter)}}$$

$$\begin{aligned}\text{amount of } KMnO_4 &= M \times \text{volume of solution} \\ &= 5.75 \times 10^{-4} \text{ mol/L} \times 500.0 \times 10^{-3} \text{ L} \\ &= 2.88 \times 10^{-4} \text{ mol}\end{aligned}$$

$$\text{mass of } KMnO_4 = 2.88 \times 10^{-4} \text{ mol} \times 158 \text{ g/mol} = 0.0454 \text{ g}$$