## **ACID-BASE EQILIBRIUM SYSTEMS**

For all the acid base equilibrium systems we can write down

- Mass balance equation
- Charge balance equation

#### **Mass Balance Equation**

#### Mass Balance Equation

The quantity of all species in a solution containing a particular atom (or group atoms) must equal the amount of that atom (or group atoms) delivered to the solution.



So the equilibrium involves the following reactions:

$$H_{2}O \longleftrightarrow H^{+} + OH^{-}$$

$$H_{3}PO_{4 (aq)} \longleftrightarrow H^{+} + H_{2}PO_{4}^{-} (aq)$$

$$H_{2}PO_{4}^{-} (aq) \longleftrightarrow H^{+} + HPO_{4}^{2-} (aq)$$

$$HPO_{4}^{2-} (aq) \longleftrightarrow H^{+} + PO_{4}^{3-} (aq)$$

 $n_{\text{H3PO4 (initial)}} = n_{\text{H3PO4 (final)}} + n_{\text{H2PO4}} + n_{\text{HPO4}} + n_{\text{PO4}}$ 1 mole

# $\frac{[H_3PO_4]_{(initial)}}{1 \text{ M}} = [H_3PO_4]_{(final)} + [H_2PO_4^{-1}] + [HPO_4^{2-1}] + [PO_4^{3-1}]$

Call  $[H_3PO_4]_{(initial)} = TOTPO_4$ 

TOTPO<sub>4</sub> = sum of the concentrations of all the species in solution that contain the chemical group  $PO_4$ .

 $TOTPO_4 = [H_3PO_4] + [H_2PO_4^{-1}] + [HPO_4^{2-1}] + [PO_4^{3-1}]$ 

#### **Mass Balance Equation**

#### Mass Balance Equation

The quantity of all species in a solution containing a particular atom (or group atoms) must equal the amount of that atom (or group atoms) delivered to the solution.

 $TOTPO_4 = [H_3PO_4] + [H_2PO_4^{-1}] + [HPO_4^{2-1}] + [PO_4^{3-1}]$ 

### **Charge Balance Equation**

Charge balance equation of any aqueous solution is:

 $n_1[C_1] + n_2[C_2] + \dots = m_1[A_1] + m_2[A_2] + \dots$ 

- C's are the concentrations of all the (+)'ly charged ions.
- n is the magnitude of the (+) charge.
- A's are the concentrations of all the (-)'ly charged ions.
- m is the magnitude of the (-) charge.

Write down the charge balance of the previous system.

Hint: Consider all the equilibrium species. Do not forget the dissociation of water.

 $H_2O \longrightarrow H^+ + OH^-$ 

 $1[H^+] = 1[H_2PO_4^-] + 2[HPO_4^2^-] + 3[PO_4^3^-] + 1[OH^-]$ 

1 mol of  $Na_2SO_4$  is added into 1 L DI water. Write down the mass balance and charge balance equations.

 $Na_2SO_{4(s)} \longrightarrow 2Na^+_{(aq)} + SO_4^{2-}_{(aq)}$ initial 1 mol - after - 2 mol 1 mol dissoc. We start with 1 M Na\_2SO\_4 \longrightarrow 2 M Na^+ and 1 M SO\_4^{2-}

[Na<sup>+</sup>] = 2 [SO<sub>4</sub><sup>2-</sup>]

Mass balance between Na<sup>+</sup> and SO<sub>4</sub><sup>2-</sup>

#### **Charge Balance Equation**

To write down the charge balance equation we have to consider the dissociation of water also.

$$H_2O \longrightarrow H^+ + OH^-$$

$$[H^+] + [Na^+] = 2 [SO_4^{2-}] + [OH^-]$$

Add 1 mol of  $Na_2CO_3$  into 1 L DI water. Write down the mass balance and charge balance equations for this solution.

Equilibrium reactions are  $Na_2CO_{3(s)} \longrightarrow 2Na^+(aq) + CO_3^2^-(aq)$   $H_2CO_3(aq) \iff H^+ + HCO_3^-(aq)$   $HCO_3^-(aq) \iff H^+ + CO_3^2^-(aq)$  $H_2O \iff H^+ + OH^-$ 

## Mass Balance Eq'n $[Na^+] = 2 [CO_3^{2-}]$ (initial) $[CO_3^{2-}]$ (initial) = TOTCO\_3 $TOTCO_3 = [CO_3^{2-}]_{(final)} + [HCO_3^{-}] + [H_2CO_3]$ $[Na^+] = 2 \{ [CO_3^2] + [HCO_3] + [H_2CO_3] \}$ MB: <u>Charge Balance Eq'n</u> CB: $[H^+] + [Na^+] = 2 [CO_3^2] + [HCO_3] + [OH^-]$

#### **Equilibrium reactions are**

 $Na_{2}CO_{3(s)} \longrightarrow 2Na^{+}(aq) + CO_{3}^{2}(aq)$   $H_{2}CO_{3(aq)} \longleftrightarrow H^{+} + HCO_{3}^{-}(aq)$   $HCO_{3}^{-}(aq) \longleftrightarrow H^{+} + CO_{3}^{2}(aq)$   $H_{2}O \longleftrightarrow H^{+} + OH^{-}$ 

Add 1 mol of  $Na_3PO_4$  into 1 L DI water. Write down the mass balance and charge balance equations for this solution.

Equilibrium reactions are  $Na_3PO_{4(s)} \longrightarrow 3Na^+(aq) + PO_4^{3-}(aq)$   $H_3PO_4(aq) \longleftrightarrow H^+ + H_2PO_4^-(aq)$   $H_2PO_4^-(aq) \longleftrightarrow H^+ + HPO_4^{2-}(aq)$   $HPO_4^{2-}(aq) \longleftrightarrow H^+ + PO_4^{3-}(aq)$  $H_2O \longleftrightarrow H^+ + OH^-$ 

## CB: $[H^+] + [Na^+] = [H_2PO_4^-] + 2[HPO_4^2^-] + 3[PO_4^3^-] + [OH^-]$

#### Charge Balance Eq'n

MB:  $[Na^+] = 3\{ [H_3PO_4] + [H_2PO_4^-] + [HPO_4^2^-] + [PO_4^3^-] \}$ 

 $TOTPO_4 = [H_3PO_4] + [H_2PO_4] + [HPO_4^2] + [PO_4^3]$ 

[PO<sub>4</sub><sup>3-</sup>]<sub>(initial)</sub> = TOTPO<sub>4</sub>

 $[Na^+] = 3 [PO4^{3}-](initial)$ 

Mass Balance Eq'n

#### **Equilibrium reactions are**

$$Na_{3}PO_{4(s)} \longrightarrow 3Na^{+}(aq) + PO_{4}^{3}(aq)$$

$$H_{3}PO_{4}(aq) \longleftrightarrow H^{+} + H_{2}PO_{4}^{-}(aq)$$

$$H_{2}PO_{4}^{-}(aq) \longleftrightarrow H^{+} + HPO_{4}^{2}^{-}(aq)$$

$$HPO_{4}^{2}(aq) \longleftrightarrow H^{+} + PO_{4}^{3}(aq)$$

$$H_{2}O \longleftarrow H^{+} + OH^{-}$$

Add 1 mol of  $Na_2HPO_4$  into 1 L DI water. Write down the mass balance and charge balance equations for this solution.

Equilibrium reactions are  $Na_2HPO_4(s) \longrightarrow 2Na^+(aq) + HPO_4^{2-}(aq)$   $H_3PO_4(aq) \longleftrightarrow H^+ + H_2PO_4^-(aq)$   $H_2PO_4^-(aq) \longleftrightarrow H^+ + HPO_4^{2-}(aq)$   $HPO_4^{2-}(aq) \longleftrightarrow H^+ + PO_4^{3-}(aq)$  $H_2O \longleftrightarrow H^+ + OH^-$ 

CB:  $[H^+] + [Na^+] = [H_2PO_4^-] + 2[HPO_4^2^-] + 3[PO_4^3^-] + [OH^-]$ 

#### <u>Charge Balance Eq'n</u>

MB:  $[Na^+] = 2\{ [H_3PO_4] + [H_2PO_4^-] + [HPO_4^2^-] + [PO_4^3^-] \}$ 

 $TOTPO_4 = [H_3PO_4] + [H_2PO_4] + [HPO_4^2] + [PO_4^3]$ 

[HPO<sub>4</sub><sup>2-</sup>](initial) = TOTPO<sub>4</sub>

 $[Na^+] = 2 [HPO4^{2}](initial)$ 

Mass Balance Eq'n

Add 1 mol of  $NaH_2PO_4$  into 1 L DI water. Write down the mass balance and charge balance equations for this solution.

Equilibrium reactions are  $NaH_2PO_{4(s)} \longrightarrow Na^{+}(aq) + H_2PO_{4^{-}(aq)}$   $H_3PO_{4(aq)} \longleftrightarrow H^{+} + H_2PO_{4^{-}(aq)}$   $H_2PO_{4^{-}(aq)} \longleftrightarrow H^{+} + HPO_{4^{2^{-}}(aq)}$   $HPO_{4^{2^{-}}(aq)} \longleftrightarrow H^{+} + PO_{4^{3^{-}}(aq)}$  $H_2O \longleftrightarrow H^{+} + OH^{-}$ 

#### CB: $[H^+] + [Na^+] = [H_2PO_4^-] + 2[HPO_4^2^-] + 3[PO_4^3^-] + [OH^-]$

#### Charge Balance Eq'n

 $\frac{\text{Mass Balance Eq'n}}{[\text{Na}^+] = [\text{H}_2\text{PO}_4^-](\text{initial})}$  $[\text{H}_2\text{PO}_4^-](\text{initial}) = \text{TOTPO}_4$  $\text{TOTPO}_4=[\text{H}_3\text{PO}_4] + [\text{H}_2\text{PO}_4^-] + [\text{HPO}_4^{2-}] + [\text{PO}_4^{3-}]$  $\text{MB:} \qquad [\text{Na}^+] = [\text{H}_3\text{PO}_4] + [\text{H}_2\text{PO}_4^-] + [\text{HPO}_4^{2-}] + [\text{PO}_4^{3-}]$