**Chemical Equilibrium and the Carbonate System**

Chemical Equilibrium

The following chemical reaction will result in the equilibrium expression given below.



**Note;**

* The species in [] are given as activities, and we will assume activity equals concentration to simplify the example.
* The activity of pure a solid or a pure liquid in an equilibrium expression has the value of one (1).

Carbonate System

Carbon dioxide in the atmosphere is in equilibrium with carbonate species in the aqueous and solid phases. Equilibrium is defined from the following basic chemical reactions. The equilibrium constants given below are at 25°C



**Closed System**

The carbonate system represented in the graph (below) is only in the aqueous phase (water). The total amount of carbonate is fixed and is split between the three aqueous species. Equations 2, 3 and 5 define the system along with a mass balance for total carbonate and a charge balance.



Note:

* At a pH <6.35, the dominant species is carbonic acid (H2CO3).
* At a pH > 6.35 and < 10.35, the dominant species is the bicarbonate (HCO3-) ion.
* At a pH > 10.35, the dominant species is the carbonate (CO3 2-) ion



**Open System**

The carbonate system represented in the graph (below) is an aqueous phase (water) in contact with a gas phase. The total amount of all carbonate species (Ct ) is relatively constant below pH approx. 6 and a function of pH > 6. Equations 1, 2, 3 and 5 define the system along with a mass balance for total carbonate that is a function of pH. The following relationship defines the total amount in the aqueous phase;



Note (as above in the closed system):

* At a pH <6.35, the dominant species is carbonic acid (H2CO3).
* At a pH > 6.35 and < 10.35, the dominant species is the bicarbonate (HCO3-) ion.
* At a pH > 10.35, the dominant species is the carbonate (CO3 2-) ion
* Current *PCO2* concentration is 10-3.5 atmospheres. Therefore based on Eq (1), H2CO3  must be equal to 10-5 M (log C = -5)



**Logarithmic Properties**

A logarithm is an exponent.

y = logbx if and only if by = x,

where;

* B is the Base
* Y is the logarithm or exponent
* x is a number given x > 0, b > 0, and b ≠1.

logb(xy) = logbx + logby.

logb(x/y) = logbx - logby.

logb(xn) = n logbx.

logbx = logax / logab.



**Logs we use**

log10 X = log X -- This is base 10 log

loge X = ln X -- This is the natural log

Log X = ln X /ln 10 -- ln 10 = 2.303

pX=-logX

Examples;

* pH = - log [H+]
* pK = - log K