18.9 SILLÈN DIAGRAM FOR CO$_2$

Partial Pressure of CO$_2$ $y_{CO2}P$= 0.5 bar.

     find pH of solution
     and concentrations.

Sillèn Diagram for fixed partial pressure of CO$_2$.

Diagram quite different from Example 18.5 when partial pressure is fixed.

Step 1: [H$^+$] and [OH$^-$] lines.
Step 2: Material Balance

$$K_{H,CO2} = 0.035 \frac{\text{mol}}{\text{kg} - \text{bar}} = \frac{a_{CO2,T}}{y_{CO2}P}$$

$$K_{H,CO2}(y_{CO2}P) = a_{CO2,T} = [CO_2]_T = [CO_2] + [H_2CO_3]$$

$$0.035(0.5) = 0.0175 \ \text{M} = [CO_2]_T$$

$$\boxed{\log(0.0175) = -1.757 = \log[CO_2]_T}$$

Sillèn Diagram

Step 3: Equilibria Constraints
    Table 18.2, E.4

$$pK_{a,1} = 6.351 \qquad K_{a,1} = \frac{[HCO_3^-][H^+]}{[CO_2]_T}$$

$$\log K_{a,1} = \log[HCO_3^-] + \log[H^+] - \log[CO_2]_T$$

$$pK_{a,2} = 10.33 \quad K_{a,2} = \frac{[CO_3^{2-}][H^+]}{[HCO_3^-]}$$

$$\log K_{a,2} = \log[CO_3^{2-}] + \log[H^+] - \log[HCO_3^-]$$

Sillèn Diagram

Step 4: Electroneutrality

Step 5: Diagram

Step 6: Proton condition