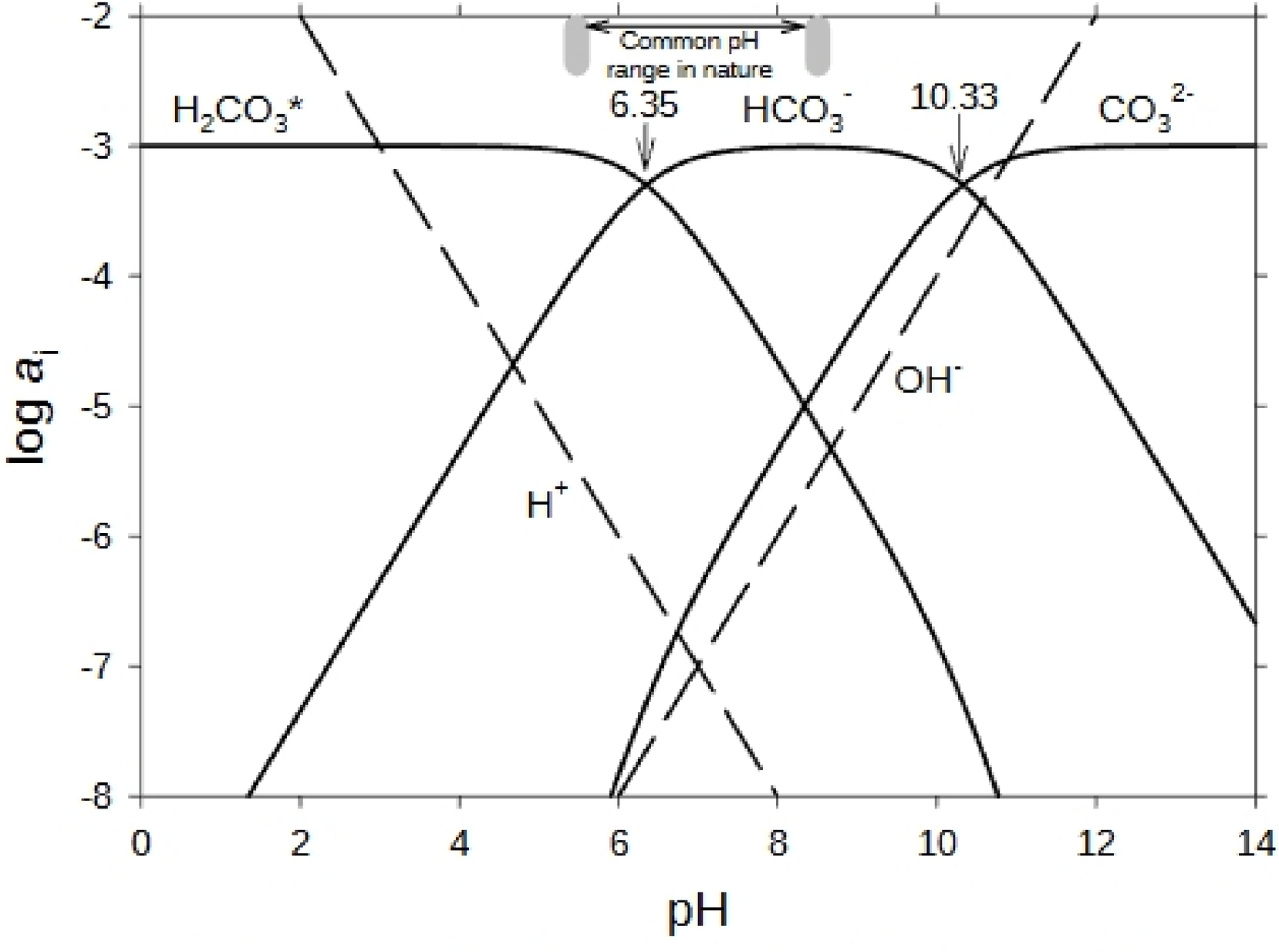
Bjerrum plot showing the activities of inorganic carbon species as a function of pH for a value of total inorganic carbon of 10^{-3} mol L^{-1}.



In most natural waters, bicarbonate is the dominant carbonate species!

SPECIATION IN OPEN CO_2-H_2O SYSTEMS - I

- In an open system, the system is in contact with its surroundings and components such as CO_2 can migrate in and out of the system. Therefore, the total carbonate concentration will not be constant.
- Let us consider a natural water open to the atmosphere, for which $p_{CO_2} = 10^{-3.5}$ atm. We can calculate the concentration of $H_2CO_3^*$ directly from K_{CO_2}:

$$K_{CO_2} = \frac{M_{H_2CO_3^*}}{p_{CO_2}} \qquad M_{H_2CO_3^*} = p_{CO_2} K_{CO_2}$$

$$\log M_{H_2CO_3^*} = \log p_{CO_2} + \log K_{CO_2}$$

Note that M_{H2CO3*} is independent of pH!

SPECIATION IN OPEN CO_2-H_2O SYSTEMS - II

- The concentration of HCO_3^- as a function of pH is next calculated from K_1:

$$K_1 = \frac{M_{HCO_3^-} a_{H^+}}{M_{H_2CO_3^*}} \qquad M_{HCO_3^-} = \frac{K_1 M_{H_2CO_3^*}}{a_{H^+}}$$

but we have already calculated $M_{H_2CO_3^*}$:

$$M_{H_2CO_3^*} = p_{CO_2} K_{CO_2}$$

so

$$M_{HCO_3^-} = \frac{K_1 K_{CO_2} p_{CO_2}}{a_{H^+}}$$

$$\log M_{HCO_3^-} = \log\left(K_1 K_{CO_2} p_{CO_2}\right) + pH$$