Speciation of inorganic carbon in aqueous solution

CO_2 dissolves in water:

(a) $CO_2(g) \rightarrow CO_2(aq)$ (same as $CO_2 \cdot H_2O$)

Dissolved CO_2 and water react to form carbonic acid:

(b) $CO_2(aq) + H_2O \rightarrow H_2CO3$ $\qquad K=10^{-2.5}$ to 10^{-3}

The small value of K means that equilibrium is far to the left in Reaction b. Thus most $CO_2(aq)$ stays as $CO_2(aq)$ - most remains as the hydrated linear CO_2 molecule (see below) rather than becoming a planar triangular CO_3^{2-} ion complexed with two H^+s. Most geochemists simplify by lumping the hydrated CO_2 and the true H_2CO_3 as H_2CO_3*:

$$[H_2CO_3^*] = [CO_2(aq)] + [H_2CO_3]$$

Thus we usually write a third equation that combines (a) and (b):

(c) $CO_2(g) + H_2O \rightarrow H_2CO_3^*$ $\qquad K_{CO2} = \dfrac{aH_2CO_3^*}{PCO_2} \overset{\text{At } 20°C}{=} 10^{-1.5}$

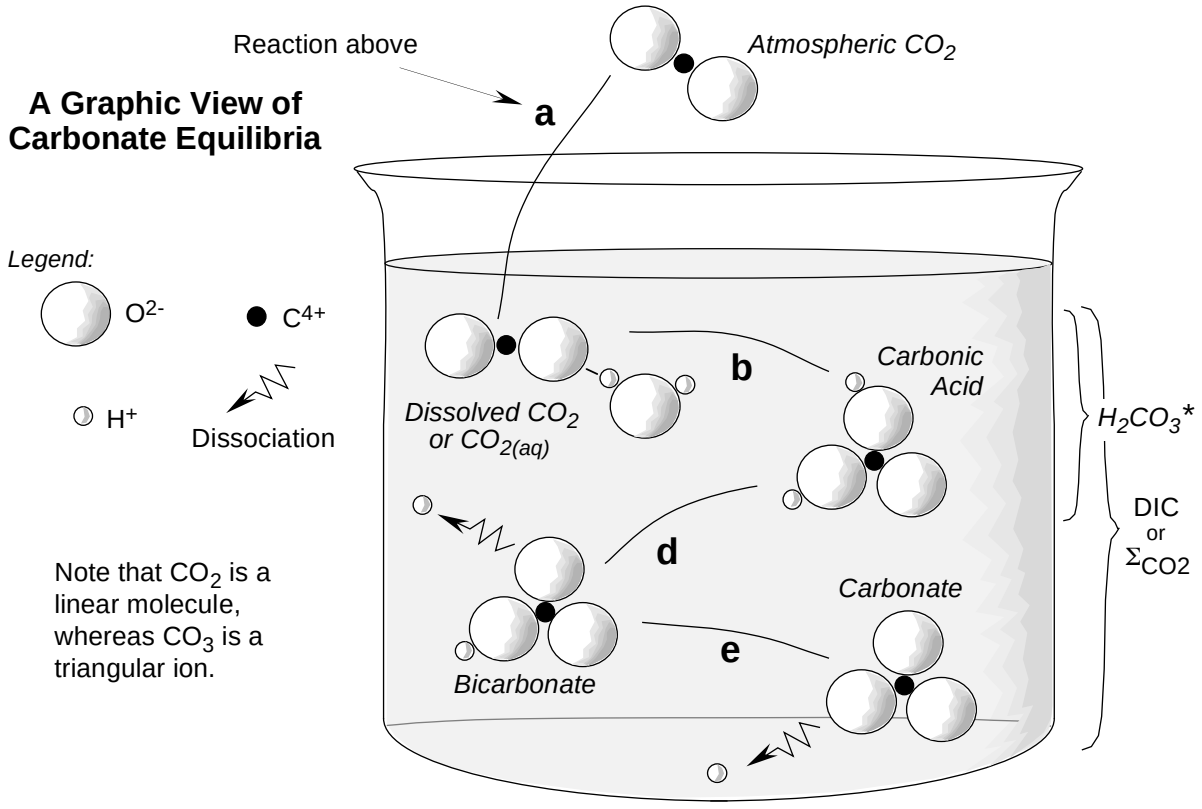
The carbonic acid can dissociate to give bicarbonate:

(d) $H_2CO_3^* \rightarrow H^+ + HCO_3^-$ $\qquad K_1 = \dfrac{aH^+ \cdot aHCO_3^-}{aH_2CO_3^*} = 10^{-6.4}$

And bicarbonate can dissociate to give carbonate:

(e) $HCO_3^- \rightarrow H^+ + CO_3^{2-}$ $\qquad K_2 = \dfrac{aH^+ \cdot aCO_3^{2-}}{aHCO_3^-} = 10^{-10.4}$

The presence of H^+ as a product in d and e means that both reactions proceed to the right much more at higher pH.



The size of the H^+ ion is greatly exaggerated relative to the other species.