

Positively charged molecular ion

Generally assume molecule



produced by



thus assuming

$$I(c) \leq I(A, B, C, \dots \text{etc})$$

and $c \geq ch$

(could be generalised to $c > ch$ easily, but rare I guess)

The code tries to construct P_N ← species of interest
in terms of atomic partial pressures

$$P_N = P_A^a P_B^b P_C^c \dots P_L^e \cdot \frac{P_{A_a B_b C_c \dots L_{e^{ch}}}}{P_A^a P_B^b P_C^{c-ch} \dots P_L^e \cdot P_{C^+}^{ch}} \cdot \frac{IT}{P_e^{ch}}$$

$$KT^{-1} = \frac{1}{PK_{diss}}$$

$$= \frac{P_C^{ch}}{P_{C^+}^{ch}} \cdot \underbrace{P_{A_a B_b C_c \dots L_{e^{ch}}}} \cdot \frac{IT}{P_e^{ch}}$$

this is what we want

So need

$$IT = P_e^{ch} \cdot \frac{P_{C^+}^{ch}}{P_C^{ch}}$$

Negative Molecular Ion

Assume molecule



produced by



thus assuming

$$I(C^-) > I(A^-, B^-, \text{etc})$$

$$\text{and } c \geq |ch| \quad \text{but } ch < 0$$

Construct P_N in code

$$P_N = P_A^a P_B^b P_C^c \dots P_L^l \cdot \underbrace{\frac{P_{A_a B_b C_c \dots L_e^{ch}}}{P_A^a P_B^b P_C^{c-|ch|} \dots P_L^l P_{C^-}^{|ch|}}}_{KT^{-1} = 1/P_{K_{diss.}}} \cdot \frac{IT}{P_e^{ch}}$$

$$= \frac{P_C^{|ch|}}{P_{C^-}^{|ch|}} \cdot P_{A_a B_b C_c \dots L_e^{ch}} \cdot \frac{IT}{P_e^{ch}}$$

so need

$$IT = P_e^{ch} \cdot \frac{P_{C^-}^{|ch|}}{P_C^{|ch|}}$$

so one could write in general

$$IT = P_e^{ch} \cdot \frac{P_{c^{ion}}^{|ch|}}{P_c^{|ch|}}$$

$$\text{where } c^{ion} = C^{\frac{ch}{|ch|}}$$

$$\text{i.e.} = C^+ \text{ if } ch > 0$$

$$= C^- \text{ if } ch < 0$$

$$\text{either if } ch = 0$$

$$\text{eg } H_2^+ \quad IT = P_e \cdot \frac{P_{H^+}}{P_H}$$

$$H_2^- \quad IT = P_e^{-1} \cdot \frac{P_{H^-}}{P_H}$$

$$H_3^+ \quad IT = P_e \cdot \frac{P_{H^+}}{P_H}$$

$$NO^+ \quad IT = P_e \cdot \frac{P_{O^+}}{P_O} \quad I(O) < I(N)$$

$$CH^- \quad IT = P_e^{-1} \cdot \frac{P_{C^-}}{P_C} \quad I(C^-) > I(H^-)$$