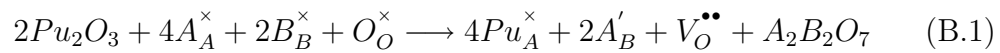# Appendix B

Normalisation of Solution Mechanisms

Here is an example of using mass action analysis for the simple solution of Pu$_2$O$_3$ onto both the A site of a pyrochlore.

$$2Pu_2O_3 + 4A_A^\times + 2B_B^\times + O_O^\times \longrightarrow 4Pu_A^\times + 2A_B' + V_O^{\bullet\bullet} + A_2B_2O_7 \qquad \text{(B.1)}$$

$$\left[Pu_A^\times\right]^4 \left[A_B'\right]^2 \left[V_O^{\bullet\bullet}\right] = \exp\left(\frac{\Delta H_{sol}}{kT}\right) \qquad \text{(B.2)}$$

From charge neutrality:

$$\left[Pu_A^\times\right] = 2\left[A_B'\right] = 4\left[V_O^{\bullet\bullet}\right] \qquad \text{(B.3)}$$

Substituting equation B.3 into equation B.2

$$\left[Pu_A^\times\right]^4 \frac{1}{4} \left[Pu_A^\times\right]^2 \frac{1}{4} \left[Pu_A^\times\right] = \exp\left(\frac{\Delta H_{sol}}{kT}\right) \tag{B.4}$$

$$\frac{1}{16}\left[Pu_A^\times\right]^7 = \exp\left(\frac{\Delta H_{sol}}{kT}\right) \tag{B.5}$$

$$\left[Pu_A^\times\right] = 16^{-7} \exp\left(\frac{\Delta H_{sol}}{7kT}\right) \tag{B.6}$$

Therefore the normalisation factor is 7.