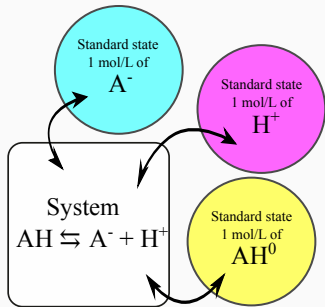


Grand-reaction ensemble.



Reaction ensemble

The reaction of an acidic unit



$$\Omega = E - TS + \sum_i (\mu_i - \mu_i^\ominus) N_i$$

Then the change of system free energy during a single reaction step

$$\Delta\Omega = k_B T \ln \left(\prod_i V^{\nu_i \xi} \frac{N_i!}{(N_i + \nu_i \xi)!} \right) + \xi \left(\sum_i \nu_i \mu_i - \sum_i \nu_i \mu_i^\ominus \right) + \Delta E$$

accept if $\mathcal{R}^\xi < e^{\Delta\Omega/k_B T}$