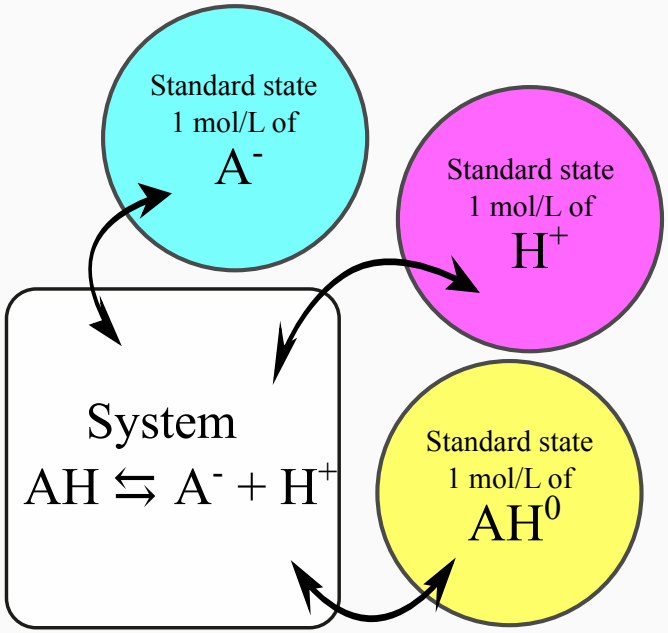
Grand-reaction ensemble.



Reaction ensemble

The reaction of an acidic unit

$$\mathrm{HA} \overset{K}{\leftrightarrows} \mathrm{A}^- + \mathrm{H}^+$$

$$\Omega = E - TS + \sum_i \left(\mu_i - \mu_i^{\ominus}\right) N_i$$

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