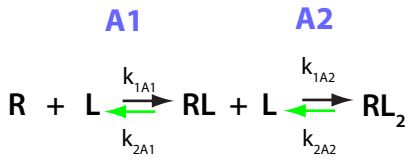
Model code: B
Binding of two ligand molecules to one receptor monomer

NOTE 1: Capital letters indicate equilibrium constants; lower case letters--kinetic constants.
NOTE 2: I use new naming of the microscopic constants, different from LineShapeKin Simulation.
NOTE 3: Isomerization transition was renamed to "B" (1/13/2015)

B_macro (macroscopic constants)

when we cannot discriminate two single-bound species



$K_{A1}=k_{1A1}/k_{2A1}$

$K_{A2}=k_{1A2}/k_{2A2}$

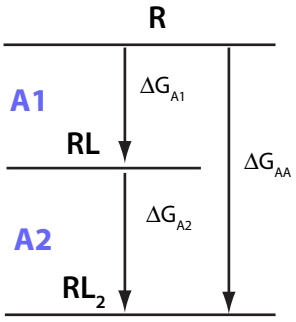
Thermodynamic cycle

$\Delta G^{o}_{AA} = \Delta G^{o}_{A1} + \Delta G^{o}_{A2}$

$K_{AA}=K_{A1}K_{A2}$

Free-energy diagram

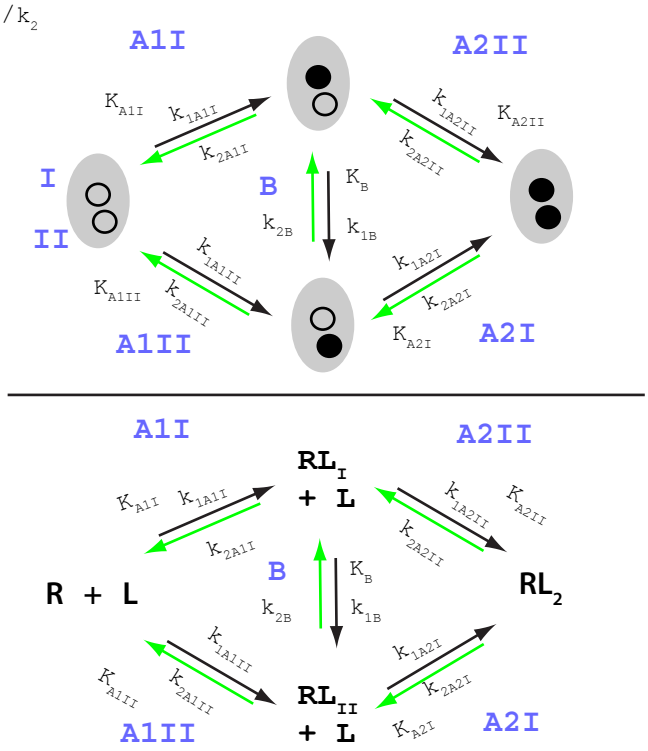
(positions of energy levels are chosen for easy viewing)



B_micro (microscopic constants)

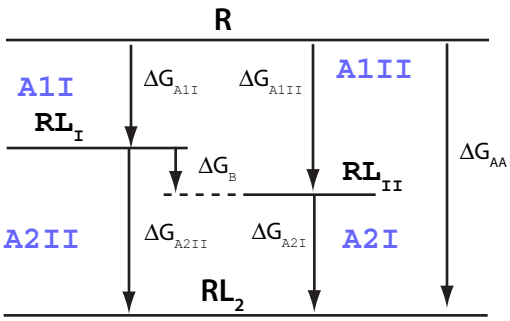
- two sites are named I and II;
- ligand-binding transitions are A1 and A2;
- B - internal isomerization transition ("hopping" inside the "solvent cage")

$K=k_1/k_2$



Free-energy diagram

(positions of energy levels are chosen for easy viewing)



Thermodynamic cycle

$\Delta G^{o}_{AA} = \Delta G^{o}_{A1I} + \Delta G^{o}_{A2II} = \Delta G^{o}_{A1II} + \Delta G^{o}_{A2I} \Rightarrow K_{AA} = K_{A1I}K_{A2II} = K_{A1II}K_{A2I}$

Dependent constants:

$\Delta G^{o}_{A2I} = \Delta G^{o}_{A1I} + \Delta G^{o}_{A2II} - \Delta G^{o}_{A1II} \Rightarrow K_{A2I} = K_{A1I}K_{A2II}/K_{A1II}$

$\Delta G^{o}_{B} = \Delta G^{o}_{A1II} - \Delta G^{o}_{A1I} \Rightarrow K_{B} = K_{A1II}/K_{A1I}$