ΔG°_{rxn} for a reaction can be calculated from ΔG°_f values

$$\Delta G^\circ_{rxn} = \sum n_{prod.} \Delta G^\circ_{f\,prod.} - \sum n_{react} \Delta G^\circ_{f\,react}$$

(n = stoichiometric coefficients)

Ex: Calculate free energy change for the rxn:

$$CH_3CH_2OH(l) + 3O_2(g) \rightarrow 2CO_2(g) + 3H_2O(l)$$

The std free energies are:

$CO_2 = -394.4$ kJ/mol

$H_2O(l) = -237.2$ kJ/mol

$CH_3CH_2OH = -174.9$ kJ/mol

$$\Delta G_{rxn} = \sum n \Delta G^\circ_f (prods) - \sum n \Delta G^\circ_f (react)$$

$$= 2\,mol(-394.4) + 3\,mol(-237.2\ kJ/mol)$$

$$-((+1)(-174.9\ kJ/mol) + 3(0))$$

$$= -1325.5\ kJ$$

Non-standard conditions

- Under non-std conditions, free energy change can be found from:

$$\Delta G = \Delta G^\circ + RT \ln Q$$

Q = react quotient

if $Q = K \Rightarrow$ at equilibrium $\Rightarrow \Delta G = 0$

$$0 = \Delta G^\circ + RT \ln K$$

$$\Delta G^\circ = -RT \ln K \quad \text{at equilib.}$$

$$K = e^{-\Delta G^\circ / RT}$$

Ex: calc. the ΔG° and K at 298K for

$$2NO(g) + Cl_2(g) \rightleftharpoons 2NOCl(g)$$

The ΔG°_f values are:

$NOCl = 66.07$ kJ/mol

$NO = 86.6$ kJ/mol

$$\Delta G^\circ = 2\,mol(66.07\ kJ/mol) - (2\,mol(86.6\ kJ/mol) + 0)$$

$$= -41.06\ kJ \times 1000\ J/kJ = -41060$$

$$K = e^{-\Delta G^\circ / RT} = e^{-(41060\ J / 8.314\ J/mol\,K)(298K)}$$

$$= 1.58 \times 10^7$$

$K > 1 \Rightarrow$ products favored, process spont.