Class example 1/22/08 ESGN541

to calculate free energy at std. conditions (ΔG_r^0) from free energy based on Table 2.2-2.4 values ($\Delta G_r^{0'}$) use the following relationship

$$\Delta G_r^0 = \Delta G_r^{0'} - RT\, \underset{\uparrow}{\upsilon_{H+}} \ln[10^{-7}]$$

stoichiometric coefficient of H+ in the reaction. the sign depends on whether it appears on the product (+) or reactant (−) side of the overall rxn

$$\Delta G_r^0 = -113.55 \frac{kJ}{e^- eq} - \left(8.314 \frac{J}{°K\text{-mol}}\right)\underset{\substack{\uparrow \\ 25°C \\ \text{std. cond.}}}{(298°K)}\left(\frac{kJ}{1000 J}\right)\left(-\frac{1}{5}\right)\ln\left[10^{-7}\right]$$

$$= -113.55 \frac{kJ}{e^- eq} - 7.99 \frac{kJ}{e^- eq} = -121.54 \frac{kJ}{e^- eq}$$

suppose we want to look at non-standard conditions

$$\Delta G_r = \Delta G_r^0 + RT \sum_{i=1}^{n} \upsilon_{ir} \ln a_i$$

use molar concentration or partial pressures for constituents of interest. use 1 for water.

$$\text{note: } \overset{\swarrow \text{sum}}{\sum_{i=1}^{n}} \upsilon_{ir} \ln a_i = \sum_{i=1}^{n} \ln a_i^{\upsilon_{ir}} = \ln \overset{\swarrow \text{product}}{\prod_{i=1}^{n}} a_i^{\upsilon_{ir}} \Leftarrow \text{log identities from long ago math class}$$

Let's look at

glucose = 100 $\frac{mg}{L}$

nitrate = 20 $\frac{mg}{L}$

mile high elevation = .82 atm

pH = 7.5

T = 15°C

N_2 = 78%

CO_2 = .03%

first convert to atm or moles

glucose = $\frac{100\,mg}{L} \times \frac{mol}{180000\,mg\ glucose} = 5.56\times10^{-4}\ \frac{mol}{L}$

nitrate = $20\,\frac{mg}{L} \times \frac{mol}{62000\,mg\ nitrate} = 3.23\times10^{-4}\ \frac{mol}{L}$

$H^+ = 10^{-7}\ \frac{mol}{L}$

H_2O = 1 (by convention for water as solvent)

N_2 = .78 × .82 atm = .64 atm

CO_2 = .0003 × .82 atm = 2.5×10^{-4} atm

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$$\Delta G_r = -121.54 \frac{kJ}{e^- eq} + RT \ln \left\{ \frac{[CO_2]^{1/4}[H_2O]^{7/20}[N_2]^{1/10}}{[C_6H_{12}O_6]^{1/24}[NO_3^-]^{1/5}[H+]^{1/5}} \right\}$$

$$\Delta G_r = -121.54 \frac{kJ}{e^- eq}$$

$$+ \left(8.314 \times 10^{-3} \frac{kJ}{°K \cdot mol}\right)(288°K) \ln \left\{ \frac{[2.4 \times 10^{-4}]^{1/4}[1]^{7/20}[.64]^{1/10}}{[5.56 \times 10^{-4}]^{1/24}[3.23 \times 10^{-4}]^{1/5}[10^{-7.5}]^{1/5}} \right\}$$

$$= -121.54 \frac{kJ}{e^- eq} + 2.39 \ln \left\{ \frac{(.124)(1)(.96)}{(.732)(.200)(.037)} \right\}$$

$$\Downarrow$$

$$21.98$$

$$= (-121.54 + 7.39) \frac{kJ}{e^- eq}$$

$$= -114.2 \frac{kJ}{e^- eq}$$