Homework #2

Due: May 07 (Thu) 23:59

Question set I: Redox reactions

In this example question, we will compare the energy obtained by aerobic oxidation of glucose ($C_6H_{12}O_6$) and nitrification ($NH_4^+ \rightarrow NO_3^-$). In both processes, microorganisms use molecular oxygen (O_2) dissolved in water as an electron acceptor.

1) Pick up a pair of half reactions from Table 14.2 of the EOC textbook for each process. Combine the half reactions to write up the overall reaction for each process and calculate the $\Delta_r G^0(W)$ values. (10 points)

2) From the E_H^0 values of the half reactions, obtain the standard free energy change ($\Delta_r G^0$) of the half reactions. From the $\Delta_r G^0$ values for half reactions, calculate the standard free energy change of the two overall reactions. (15 points)

3) Assume you added 90 mg/L glucose and 14 mg-N/L NH_4^+ into water at 25℃ and pH=7.0. You maintained the dissolved oxygen (DO) concentration in the water as 8 mg/L and inoculated a group of microorganisms that mediate either of the two reactions. Calculate the $\Delta_r G$ values for both reactions. Assume the partial pressure of CO_2 as 3.0×10^{-4} atm and NO_3−N concentration of 0.1 mM. (15 points)

(Hint: assume molarity (M) equals activity for dissolved constituents. For gas constituents, use partial pressure as activity. Assume activity of water as 1.)

4) In the condition given in 3), which process is more competitive, glucose oxidation or nitrification? Can you guess how the glucose and ammonium concentration will change over time? (10 points)

Question set II: Nucleophilic reactions

Following concentrations for anionic constituents are determined for a water sample with a pH value of 7.0 at 25℃.

Constituents	Ionic weight	Concentration (mg/L)
NO_3^-	62.0	27.2
SO_4^{2-}	96.1	76.5
Cl^-	35.5	204.7
OH^-	17.0	can be derived from pH

The n_{Nu,CH_3Br} values for the anions are shown below:

Anionic nucleophiles	n_{Nu,CH_3Br}
NO_3^-	1.0
SO_4^{2-}	2.5
Cl^-	3.0
OH^-	4.2

1) Determine the $[Nu]_{50\%}$ values for the anionic nucleophiles assuming s=1. Considering the $[Nu]_{50\%}$ values and the nucleophile concentrations, list nucleophiles that are significant for reaction with CH_3Br in the water. If the reaction rate for a nucleophile is more than 5% of the hydrolysis rate, determine the nucleophile as significant. (20 points)

2) If 10^{-5} M of CH_3Br is added to the water sample, what will be the concentration of the products of nucleophilic substitution (including hydrolysis) after all the reactions occur completely? Consider only significant nucleophiles. (30 points)