Assignment #4: Chemical Kinetics of Aspirin Hydrolysis

Experimental data are provided on the back of the page. To guide your review of chemical kinetics, two links are provided on the "Assignments" page of the course web site.

(a) Determination of the Order of Reaction (Sheet #1). Enter the data for experiment #1 on sheet #1 in columns A and B, compute the values of ln[Aspirin]) and 1/[Aspirin]) in columns C and D, and create marked (X,Y) scatter plots for (*t*, [Aspirin]), (*t*, ln[Aspirin]), and (*t*, 1/[Aspirin]). What is the order of the reaction?

(b) Determination of the Reaction Rate Constants *k'* and *k* (Sheet #2). Copy appropriate data from sheet #1. Pseudo-first-order kinetics apply, i.e., [aspirin] = $[\text{aspirin}]_0 \exp(-k't)$ and $\ln[\text{aspirin}] = \ln[\text{aspirin}]_0 - k't$, and $k = k'/55.55$. Determine the pseudo-first-order reaction rate constant *k'* in three ways: [1] One commonly determines the rate constant *k* as the slope of the linear regression of the (*t*, ln[Aspirin]) scatter plot. [2] Alternatively, one can directly fit an exponential function to the (*t*, [Aspirin]) data. [3] Use the excel function SLOPE and the (*t*, ln[Aspirin]) data. With the concentration of water (55.55 mol/L), also determine the second-order rate constant $k = k'/55.55$. Report *k'* and *k* with the appropriate units.

(c) Determination of the Activation Parameters (Sheet #3). Enter the data of experiment #2 on sheet #3 in columns A and B. Use the Arrhenius and Eyring equations to determine the activation parameters E_{act}, H_{act} and S_{act} and report the resulting values with the correct units.

Submission & Deadline: The assignment must be completed with MS Excel 2007. Submit one Excel file "A4_'your name'.xlsx" with **(a)** on sheet #1, **(b)** on sheet #2, and **(c)** on sheet #3 by Tuesday, 02/23/10, midnight. Bring one hardcopy to class on Wednesday, 02/24/10.

Table 1. Measured Data from Experiment #1. Concentrations of aspirin measured as a function of time at 39 °C after one tablet (335 mg) of aspirin was dissolved in 1 L water. MM(aspirin) = 180.157 g/mol.

t [sec]	[aspirin] [mmol/liter]	ln[aspirin]	1/[aspirin]
0	1.80398		
600	1.25236		
1200	0.86942		
1800	0.60357		
2400	0.41901		
3000	0.29089		
3600	0.20194		
4200	0.14019		
4800	0.09732		
5400	0.06756		
6000	0.04690		
6600	0.03256		
7200	0.02261		
7800	0.01569		
8400	0.01089		
9000	0.00756		
9600	0.00525		
10200	0.00365		
10800	0.00253		

Table 2. Measured Data from Experiment #2. Second-order reaction rate constants as a function of reaction temperature.

T [°C]	*k* [10^4 min^{-1}]	*k* [sec^{-1}]	ln[*k*]	ln[*k*/*T*]
39	6.57			
47.25	14.48			
55.1	29.18			