Chemistry 4000/5000/7000 Fall 2010 Assignment 3

Due: Friday, Oct. 1, 4:00 p.m.

Marks: 20

1. In lecture 3, we briefly encountered the mechanism of S_N1 reactions. Using the steady-state approximation and one additional assumption, show that this mechanism predicts a first-order rate law for S_N1 reactions. [10 marks]

2. A Michaelis-Menten (a.k.a. Monod) growth term is not the only possibility in a cell culture model like the one studied in lecture 6. One alternative is the Droop equation:

$$v_u = \begin{cases} 0 & \text{if } [\mathrm{G}_{(\mathrm{in})}] < G_{\min}, \\ \gamma_{\max} B \left(1 - G_{\min}/[\mathrm{G}_{(\mathrm{in})}]\right) & \text{if } [\mathrm{G}_{(\mathrm{in})}] \geq G_{\min}. \end{cases}$$

   Modify the ode file studied in class to use this growth term instead of the Michaelis-Menten form. Try to estimate the parameters. (This may require a bit of digging.) Compare the behavior of the model with Droop growth kinetics to the behavior of the original model. [10 marks]

   Note: There are at least two ways to define the above function in xppaut. There is an `if...then...else` function, with the obvious meaning. There is also a function called `heav()` that returns the Heaviside function (0 if the argument is negative, 1 otherwise).