

Chemistry 4010 Fall 2019

Test 1

Time allowed: 2 hours

Marks: 51

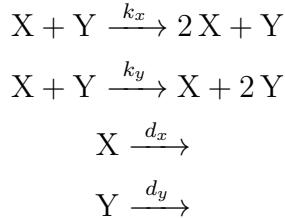
Handwritten notes are allowed. No printed or mechanically reproduced materials of any kind are permitted.

Software allowed: text editor, XPPAUT, calculator. If any other software is found to be in use during this exam, you will receive a grade of zero.

Answers are to be written in the exam booklets provided. If your answer involves the use of software, make sure to describe the calculation and to provide a reasonable sketch of any graphical results.

1. Sketch trajectories in a two-dimensional phase space near each of the **6 marks** following types of equilibrium points: [2 marks each]
 - (a) stable node
 - (b) unstable node
 - (c) saddle point
2. Sketch the bifurcation diagram for a transcritical bifurcation. Be sure **3 marks** to distinguish stable and unstable equilibria, perhaps using solid vs dashed lines, and provide a legend to indicate which line type is which. [3 marks]
3. Explain, using both text and diagrams, the difference between a super- **6 marks** critical and a subcritical Andronov-Hopf bifurcation. [6 marks]

4. The following is a simple mass-action model for a population that re- **20 marks** produces sexually:



The first two “reactions” are reproduction, producing female (X) and male (Y) offspring, respectively. The last two “reactions” represent death. One can imagine *many* improvements to such a model.

- Write down the mass-action differential equations for this model.
[4 marks]
- Determine the equilibrium points of this model. [6 marks]
- Carry out **one** of the following analyses:
 - A phase-plane analysis of the model
 - A linear stability analysis of the two equilibria

Based on your analysis, what does this model predict about the population? [10 marks]

Note: if you try both, **clearly indicate which one I am to grade**. I will **only** grade **one** solution. Absent clear directions from you, I will grade the first solution I find.

5. The peroxidase-oxidase reaction is an enzyme-catalyzed redox reaction that displays bistability in an CSTR. An early model for this reaction involved uncompetitive substrate inhibition, i.e. an unproductive ES_2 complex.¹ The overall rate equation is 16 marks

$$\frac{dS}{dt} = Q(S_0 - S) - \frac{VS}{1 + \frac{S}{K_M} + \frac{S^2}{K_M K_I}}.$$

- (a) Transform this differential equation to dimensionless form. Because we want to vary Q , *do not* use Q in the definitions of your dimensionless *variables*. [5 marks]
- (b) What is the equilibrium point when $Q = 0$? [1 mark]
- (c) Experimentally, it is easy to vary Q , which represents a pumping rate. Your dimensionless equations should contain a parameter proportional to Q . Generate a bifurcation diagram varying this parameter using AUTO, and demonstrate that there is a range of bistability. Your answer should include a sketch of the bifurcation diagram along with the values of the parameter at the two bifurcation points. Also make sure to name the type of bifurcation observed. [10 marks]

Here are some parameters you can use: $S_0 = 10 \mu\text{M}$, $V = 1 \text{ s}^{-1}$, $K_M = 1 \mu\text{M}$, $K_I = 0.5 \mu\text{M}$. You will of course have to calculate the parameters of your dimensionless representation using these.

¹Degn, *Nature* **217**, 1047.