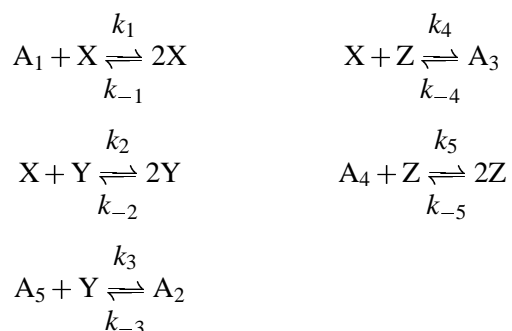# Chemistry 5850 Summer 2004 Assignment 3

Due: Thursday, May 20.

Weight of this assignment: 20 marks

Some years ago, Willamowski and Rössler constructed a model with complex behavior which (a) was fully reversible and thus consistent with thermodynamics, and (b) contained no unrealistic third- or higher-order elementary reactions [1].Their model is

$$A_1 + X \underset{k_{-1}}{\overset{k_1}{\rightleftharpoons}} 2X \qquad\qquad X + Z \underset{k_{-4}}{\overset{k_4}{\rightleftharpoons}} A_3$$

$$X + Y \underset{k_{-2}}{\overset{k_2}{\rightleftharpoons}} 2Y \qquad\qquad A_4 + Z \underset{k_{-5}}{\overset{k_5}{\rightleftharpoons}} 2Z$$

$$A_5 + Y \underset{k_{-3}}{\overset{k_3}{\rightleftharpoons}} A_2$$

The concentrations A_i are all assumed to be constant. Reduce the model to dimensionless form. Carry out a numerical survey of this model. Try to find examples of as many qualitatively different behaviors as possible.

Hint: Try $k_1 = k_2 = k_3 = k_{-3} = k_4 = k_5 = 1$, $k_{-1} = 0.25$, $k_{-2} = 10^{-3}$, $k_{-5} = 0.5$, $A_2 = A_3 = 0.01$, $A_4 = 16.5$ and $A_5 = 10$ to start. (I'm deliberately not giving you a value for A_1. Experiment!) Obviously, you should feel free to change any or all of the constants.

References

[1] K.-D. Willamowski and O. Rössler, Z. Naturforsch. A **35**, 317 (1980).