Chemical Kinetics - Reaction of Unknown Order - Two Reactants

Click on BEGIN, enter your code number, and press RETURN. The program will present a set of data at 25 C for an unknown-order reaction:

\[ \nu_A \text{A} + \nu_B \text{B} \rightarrow \text{products} \]

This set of data is produced for an initial concentrations of A and B in their stoichiometric proportion \( \{[A]_o/\nu_A = [B]_o/\nu_B\} \), with a particular time increment between readings so that the data covers approximately 75% of the reaction (about 25% of the limiting reagent remaining).

Your problem is to first determine the order (\( \alpha \)) of this reaction, then to accurately determine the rate constant (\( k \)), as in

\[ -\left(1/\nu_A\right)d[A]/dt = -\left(1/\nu_B\right)d[B]/dt = k[A]^\alpha [B]^\beta \]

The orders may be determined by any technique, but you should document the technique and the data sets you use for this determination. The orders may be determined by

1. the method of initial rates
or by

2. Do at least two of the following:
   (a) find the overall order by working with the components in their stoichiometric ratio
   (b) overload with component A to determine the value of b
   (c) overload with component B to determine the value of a

The second problem is to accurately determine the rate constant (and its uncertainty) at three different concentrations covering at least a ten-fold range of concentrations for each component. There are a few conditions in which the rate constant may be determined directly (\( \alpha = \beta = 1 \), \( \alpha = 0 \) or \( \beta = 0 \)), but usually \( k \) must be determined from \( k' \) and \( n \) or \( k'' \) and \( m \), as in

\[ -\left(1/\nu_A\right)d[A]/dt = k'[A]^n \quad \text{or} \quad -\left(1/\nu_B\right)d[B]/dt = k''[B]^m \]

The constancy of the rate constant should verify the accuracy of the orders you have determined. Report values of \( \alpha \) and \( \beta \), and the average \( k \) with its uncertainty.

Processing data.

The processing of data to determine the rate constant will depend on the orders of the reaction, as has been covered in class. To be sure that you have the correct orders, values of \( k \) should be determined for at least two of the conditions:

\( \{[A]_o/\nu_A = [B]_o/\nu_B\} \); \( \{[A]_o/\nu_A >> [B]_o/\nu_B\} \); or \( \{[A]_o/\nu_A << [B]_o/\nu_B\} \)

To be sure that you have handled the stoichiometric values (\( \nu_A, \nu_B \)) properly, you should have some calculations based on [A] vs t, and some based on [B] vs t. Hand in the data sets you have generated for determining the orders and the rate constant.