Tutorial 3

Course Coordinator: Dr. Shashank Deep

Q1. Suggest plausible mechanisms for the following reaction:

$$C(CH_3)_3Cl + OH^- \rightarrow C(CH_3)_3OH + Cl^-$$

$$\frac{-d[C(CH_3)_3Cl]}{dt} = \frac{k[C(CH_3)_3Cl][OH^-]}{k'[Cl^-] + k''[OH^-]}$$

Q3. Propose reaction steps consistent with the rate law for the hydrolysis of benzhydril chloride; relate a, b to the rate constant.

$$Ph_2CHCl + H_2O = Ph_2CHOH + Cl^- + H^+$$

$$\frac{d[Ph_2CHOH]}{dt} = \frac{\alpha[Ph_2CHCl]}{\beta + [Cl^-]}$$

Q3. Consider a simple second-order reaction

Solve the differential equation using fourth order Runge-Kutta method considering $[A]_0$ = $2.16*10^{-4}$ M and k=127.9 $Lmol^{-1}s^{-1}$ and calculate amount of reactant at 2 and 4 second.

Q4. Consider the following scheme

$$A \xrightarrow{k_1} P \qquad\qquad A + B \xrightarrow{k_2} Q$$

Calculate the concentration of A, B, P and Q at 0.8 s using fourth order Runge-Kutta method. The condition used were $[A]_0$ = 1 M, B_0 = 1.2 M, k_1 = 1 sec^{-1}, and k_2 = 2 $Lmol^{-1}s^{-1}$.