Assignment 3

1. The irreversible isomerisation reaction ($A \longrightarrow B$) was carried out in a batch reactor and the following conc.-time data were obtained.

t(min.)	0	1	2	3	4	5	6	7	8	9	10	15	20
C_A(mol/m^3)	0.041	0.034	0.027	0.023	0.021	0.018	0.016	0.015	0.0136	0.012	0.0114	0.009	0.0067

   Determine reaction order and reaction rate constant by using-
   a) Integral method.
   b) Differential method.
   c) Compare the result and comment on the methods.
2. The rate of reaction of A and B ($A+B \longrightarrow AB$), from the rate data given in table. Suggest a mechanism and rate equation for this reaction and determine the rate constant also.

Conc. of A (mole/liter)	Conc. of B (mole/liter)	Rate of reaction (mole/liter)(min^{-1})
1.0	0.02	4.6×10^{-4}
1.0	0.04	9.2×10^{-4}
0.02	1.0	9.2×10^{-6}
0.04	1.0	3.68×10^{-5}

3. Find the first order rate constant for the disappearance of A for the gas phase reaction ($2A \longrightarrow B$) occurring in a batch reactor under constant pressure condition. The volume of reaction mixture initially consists of 80% A, and decreased by 40% in 3 min.
4. Find the order of irreversible reaction from the following half-life data.

C_{A0}(mole\lit.)	5	10	15	20
$t_{1/2}$(sec)	40	20	13.5	10

   Also find the value of reaction rate constant.
5. Experimental studies for specific decomposition of A in a batch reactor using pressure units, shows exactly the same rate at two different temperatures.
   At 300K $(-r_A) = 6.7\times P_A^2$
   400K $(-r_A) = 6.7\times P_A^2$
   Where, $(-r_A)$ = mole/(m3.sec) and P_A = atm.
   a) Evaluate the activation energy using these units.
   b) transform the rate expression into concentration units and then evaluate the activation energy.
   The pressure is not excessive, so the ideal gas law can be used.

   (Note: Please plot graphs on excel sheet, where required.)