**Chemical kinetics – HL**

16.1 – Rate expression and Reaction mechanism

Rate equation

* The rate of a reaction depends on the concentration of the reactants

So, in the reaction A + B 🡪 C + D

Rate [A]

Rate [B]

Rate [A][B]

Rate = k[A][B] . . . . . . . can be expressed as rate = k[A]m[B]n

* Where m and n represent the order of the reaction with respect to the concentrations of reactant A and B respectively. The orders give an indication of how sensitive the reaction rate is to the concentration of a reactant.
* Overall order of reaction = m + n
* The value of the rate constant (k) depends on temperature and its units are determined from the overall order of the reaction
* Rate equations cannot be deduced from theory but must be determined experimentally.

**Molecularity and rate determining step of a reaction**

Reaction mechanism =

Molecularity – describes the number of particles (molecules or atoms) involved in an elementary step/reaction/process of a reaction

Unimolecular =

Bimolecular =

Termolecular =

Reaction intermediate = produced in one step and used up in a subsequent step

Rate determining step = slowest step in the reaction that limits the speed of the overall reaction

Non chemistry example –

Deduction of a rate equation from a proposed reaction mechanism

1. Decide on which step is the RDS
2. From (1) deduce the rate equation

A reaction mechanism is a hypothesis of the sequence of events that converts the reactants to the products. There may be several possible mechanisms that fit the available evidence.

Read over the worked example on pg. 379-380, then work through the following example.

Example #1

Given the following equations and experimental data, write the correct

* Rate Law Expression
* Reaction Order
* Determine k, the Specific Rate Constant (including units)

 A2 + B2 → 2 AB

|  |  |  |  |
| --- | --- | --- | --- |
| Exp # | [A2] | [B2] | Rate |
|  |  |  | (mole L-1 s-1) |
| 1 | 0.001 | 0.001 | 0.01 |
| 2 | 0.001 | 0.002 | 0.02 |
| 3 | 0.001 | 0.003 | 0.03 |
| 4 | 0.001 | 0.004 | 0.04 |
| 5 | 0.002 | 0.004 | 0.16 |
| 6 | 0.003 | 0.004 | 0.36 |

Graphical representations of zero order, first order, and second order reactions

Zero order –

First order

Second Order –

**16.2 - Activation Energy and the Arrhenius equation**

Based on kmt and collision theory, we know that certain conditions must be met for a reaction between particles (atoms/molecules) to occur.

1. Particles must \_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_
2. Particles must have correct \_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_ with respect to each other
3. Colliding particles must have sufficient \_\_\_\_\_\_\_\_\_\_\_\_\_\_ \_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_

We can summarize this as

$$k=p × Z × e^{\frac{-Ea}{RT}}$$

Look on pg. 384 to find the meaning of the terms in this expression.

Why can p and Z be grouped together as ‘A’ in the Arrhenius equation?

What does the $e^{\frac{-Ea}{RT}}$ term in the expression mean?

Write both forms of the Arrhenius equation below.

What is the advantage of taking the ln of both sides? What can a plot of lnk vs. 1/T help us to find?