Additional higher level

Topic 16: Chemical kinetics

6 hours

Essential idea: Rate expressions can only be determined empirically and these limit possible reaction mechanisms. In particular cases, such as a linear chain of elementary reactions, no equilibria and only one significant activation barrier, the rate equation is equivalent to the slowest step of the reaction.

16.1 Rate expression and reaction mechanism

Nature of science:

Principle of Occam's razor—newer theories need to remain as simple as possible while maximizing explanatory power. The low probability of three molecule collisions means stepwise reaction mechanisms are more likely. (2.7)

Understandings:

- Reactions may occur by more than one step and the slowest step determines the rate of reaction (rate determining step/RDS).
- The molecularity of an elementary step is the number of reactant particles taking part in that step.
- The order of a reaction can be either integer or fractional in nature. The order of a reaction can describe, with respect to a reactant, the number of particles taking part in the rate-determining step.
- Rate equations can only be determined experimentally.
- The value of the rate constant (k) is affected by temperature and its units are determined from the overall order of the reaction.
- Catalysts alter a reaction mechanism, introducing a step with lower activation energy.

Applications and skills:

- Deduction of the rate expression for an equation from experimental data and solving problems involving the rate expression.
- Sketching, identifying, and analysing graphical representations for zero, first and second order reactions.
- Evaluation of proposed reaction mechanisms to be consistent with kinetic and stoichiometric data.

International-mindedness:

- The first catalyst used in industry was for the production of sulfuric acid. Sulfuric acid production closely mirrored a country's economic health for a long time. What are some current indicators of a country's economic health?

Theory of knowledge:

- Reaction mechanism can be supported by indirect evidence. What is the role of empirical evidence in scientific theories? Can we ever be certain in science?

Utilization:

- Cancer research is all about identifying mechanisms; for carcinogens as well as cancer-killing agents and inhibitors.

Syllabus and cross-curricular links:
Topic 20.1—organic mechanisms especially S_N1 and S_N2
Option A.3—catalysts
Biology topic 8.1—enzymes acting as catalysts

Aims:

- **Aim 7**: Databases, data loggers and other ICT applications can be used to research proposed mechanisms for lab work performed and to carry out virtual experiments to investigate factors which influence rate equations.

16.1 Rate expression and reaction mechanism	
Guidance: • Calculations will be limited to orders with whole number values. • Consider concentration–time and rate–concentration graphs. • Use potential energy level profiles to illustrate multi-step reactions; showing the higher E_a in the rate-determining step in the profile. • Catalysts are involved in the rate-determining step. • Reactions where the rate-determining step is not the first step should be considered. • Any experiment which allows students to vary concentrations to see the effect upon the rate and hence determine a rate equation is appropriate.	

Essential idea: The activation energy of a reaction can be determined from the effect of temperature on reaction rate.

16.2 Activation energy

Nature of science:

Theories can be supported or falsified and replaced by new theories—changing the temperature of a reaction has a much greater effect on the rate of reaction than can be explained by its effect on collision rates. This resulted in the development of the Arrhenius equation which proposes a quantitative model to explain the effect of temperature change on reaction rate. (2.5)

Understandings:

- The Arrhenius equation uses the temperature dependence of the rate constant to determine the activation energy.
- A graph of *1/T* against ln *k* is a linear plot with gradient – E_a / R and intercept, ln*A*.
- The frequency factor (or pre-exponential factor) (*A*) takes into account the frequency of collisions with proper orientations.

Applications and skills:

- Analysing graphical representation of the Arrhenius equation in its linear form $\ln k = \frac{-E_a}{RT} + \ln A$.
- Using the Arrhenius equation $k = A e^{\frac{-E_a}{RT}}$.
- Describing the relationships between temperature and rate constant; frequency factor and complexity of molecules colliding.
- Determining and evaluating values of activation energy and frequency factors from data.

Guidance:

- Use energy level diagrams to illustrate multi-step reactions showing the RDS in the diagram.
- Consider various data sources in using the linear expression $\ln k = \frac{-E_a}{RT} + \ln A$. The expression $\ln \frac{k_1}{k_2} = \frac{E_a}{R}\left(\frac{1}{T_2} - \frac{1}{T_1}\right)$ is given in the data booklet.

Utilization:

- The flashing light of fireflies is produced by a chemical process involving enzymes.
- The relationship between the “lock and key” hypothesis of enzymes and the Arrhenius equation.

Syllabus and cross-curricular links:
Topic 6.1—collision theory

Aims:

- **Aims 4** and **7**: Use of simulations and virtual experiments to study effect of temperature and steric factors on rates of reaction.
- **Aim 6**: Experiments could include those involving the collection of temperature readings to obtain sufficient data for a graph.
- **Aim 7**: Graphing calculators can be employed to easily input and analyse data for E_a and frequency factor values.