Unit 7 Kinetics - Time Trials

Content Area: Science
Course(s): AP Chemistry
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Rates of reactions will change with external variable; controlling variable can produce desired results.

Enduring Understandings

The rate of a chemical reaction is influenced by controllable outside forces.

Not all reactions happen in one step.

The rate of a chemical reaction does not determine the quantity of the product.

Essential Questions

How will changing conditions affect the rate of chemical reactions?

What role does the thermodynamics of a reaction play in the kinetics?

To what extent can the rate of a reaction be predicted?

Content

Vocabulary:

Mechanism, rate determining step, catalyst, activated complex, transition state, activation energy, collision theory, intermediate, reactant order, rate law, kinetics, reaction rate, elementary step, molecularity

Use the collision theory to explain how the rate of a chemical reaction is influenced by temperature, particle size of reactants, concentration, and of the nature of the reactants.

Given a potential energy diagram, determine whether a reaction is endothermic or exothermic, determine the heat of reaction for the forward and reverse reaction. And determine the activation energy for the forward an reverse reactions (both catalyzed and uncatalyzed).

Determine the order of reactants using experimental date and write the rate law.

Express the rate of a reaction in terms of concentration variations in reactants and products.

Calculate average and instantaneous rate from a graphical relationship

Use and write reactions mechanisms, identifying intermediates, catalyst, rate determining step and writing the observed rate law.

Resources

Standards

Big Idea 4: Rates of chemical reactions are determined by details of the molecular collisions.

Enduring understanding 4.A: Reaction rates that depend on temperature and other environmental factors are determined by measuring changes in concentrations of reactants or products over time. Essential knowledge 4.A.1: The rate of a reaction is influenced by the concentration or pressure of reactants, the phase of the reactants and products, and environmental factors such as temperature and solvent.

- a. The rate of a reaction is measured by the amount of reactants converted to products per unit of time.
- b. A variety of means exist to experimentally measure the loss of reactants or increase of products as a function of time. One important method involves the spectroscopic determination of concentration through

Beer's Law.

c. The rate of a reaction is influenced by reactant concentrations (except in zero-order processes), temperature, surface area, and other environmental factors.

4.A.1 Learning Objective:

LO 4.1 The student is able to design and/or interpret the results of an experiment regarding the factors (i.e., temperature, concentration, surface area) that may influence the rate of a reaction. [See SP 4.2, 5.1]

Essential knowledge 4.A.2: The rate law shows how the rate depends on reactant concentrations.

- a. The rate law expresses the rate of a reaction as proportional to the concentration of each reactant raised to a power. The power of each reactant in the rate law is the order of the reaction with respect to that reactant. The sum of the powers of the reactant concentrations in the rate law is the overall order of the reaction. When the rate is independent of the concentration of a reactant, the reaction is zeroth order in that reactant, since raising the reactant concentration to the power zero is equivalent to the reactant concentration being absent from the rate law.
- b. In cases in which the concentration of any other reactants remain essentially constant during the course of the reaction, the order of a reaction with respect to a reactant concentration can be inferred from plots of the concentration of reactant versus time. An appropriate laboratory experience would be for students to use spectrophotometry to determine how concentration varies with time.
- c. The method of initial rates is useful for developing conceptual understanding of what a rate law represents, but simple algorithmic application should not be considered mastery of the concept. Investigation of data for initial rates enables prediction of how concentration will vary as the reaction progresses.

4.A.2 Learning Objective:

LO 4.2 The student is able to analyze concentration vs. time data to determine the rate law for a zeroth-, first-, or second-order reaction. [See SP 5.1, connects to 4.A.3]

Essential knowledge 4.A.3: The magnitude and temperature dependence of the rate of reaction is contained quantitatively in the rate constant.

- a. The proportionality constant in the rate law is called the rate constant.
- b. The rate constant is an important measurable quantity that characterizes a chemical reaction.
- c. Rate constants vary over many orders of magnitude because reaction rates vary widely.
- d. The temperature dependence of reaction rates is contained in the temperature dependence of the rate constant.
- e. For first-order reactions, half-life is often used as a representation for the rate constant because they are inversely proportional, and the half-life is independent of concentration. For example, radioactive decay processes provide real-world context.

4.A.3 Learning Objective:

LO 4.3 The student is able to connect the half-life of a reaction to the rate constant of a first-order reaction and justify the use of this relation in terms of the reaction being a first-order reaction. [See SP 2.1, 2.2]

Enduring understanding 4.B: Elementary reactions are mediated by collisions between molecules. Only collisions having sufficient energy and proper relative orientation of reactants lead to products. Essential knowledge 4.B.1: Elementary reactions can be unimolecular or involve collisions between two or more molecules.

- a. The order of an elementary reaction can be inferred from the number of molecules participating in a collision: unimolecular reactions are first order, reactions involving bimolecular collisions are second order, etc.
- b. Elementary reactions involving the simultaneous collision of three particles are rare.

4.B.1 Learning Objective:

LO 4.4 The student is able to connect the rate law for an elementary reaction to the frequency and success of molecular collisions, including connecting the frequency and success to the order and rate constant, respectively. [See SP 7.1, connects to 4.A.3, 4.B.2]

Essential knowledge 4.B.2: Not all collisions are successful. To get over the activation energy barrier, the colliding species need sufficient energy. Also, the orientations of the reactant molecules during the collision must allow for the rearrangement of reactant bonds to form product bonds.

- a. Unimolecular reactions occur because collisions with solvent or background molecules activate the molecule in a way that can be understood in terms of a Maxwell-Boltzmann thermal distribution of particle energies.
- b. Collision models provide a qualitative explanation for order of elementary reactions and the temperature dependence of the rate constant.
- c. In most reactions, only a small fraction of the collisions leads to a reaction. Successful collisions have both sufficient energy to overcome activation energy barriers and orientations that allow the bonds to rearrange in the required manner.
- d. The Maxwell-Boltzmann distribution describes the distribution of particle energies; this distribution can be used to gain a qualitative estimate of the fraction of collisions with sufficient energy to lead to a reaction, and also how that fraction depends on temperature.

4.B.2 Learning Objective:

LO 4.5 The student is able to explain the difference between collisions that convert reactants to products and those that do not in terms of energy distributions and molecular orientation. [See SP 6.2]

Essential knowledge 4.B.3: A successful collision can be viewed as following a reaction path with an associated energy profile.

- a. Elementary reactions typically involve the breaking of some bonds and the forming of new ones. It is usually possible to view the complex set of motions involved in this rearrangement as occurring along a single reaction coordinate.
- b. The energy profile gives the energy along this path, which typically proceeds from reactants, through a transition state, to products.
- c. The Arrhenius equation can be used to summarize experiments on the temperature dependence of the rate of an elementary reaction and to interpret this dependence in terms of the activation energy needed to reach the transition state.

4.B.3 Learning Objective:

LO 4.6 The student is able to use representations of the energy profile for an elementary reaction (from the reactants, through the transition state, to the products) to make qualitative predictions regarding the relative temperature dependence of the reaction rate. [See SP 1.4, 6.4]

Enduring understanding 4.C: Many reactions proceed via a series of elementary reactions. Essential knowledge 4.C.1: The mechanism of a multistep reaction consists of a series of elementary reactions that add

up to the overall reaction.

- a. The rate law of an elementary step is related to the number of reactants, as accounted for by collision theory.
- b. The elementary steps add to give the overall reaction. The balanced chemical equation for the overall reaction specifies only the stoichiometry of the reaction, not the rate.
- c. A number of mechanisms may be postulated for most reactions, and experimentally determining the dominant pathway of such reactions is a central activity of chemistry.

Essential knowledge 4.C.2: In many reactions, the rate is set by the slowest elementary reaction, or rate-limiting step.

a. For reactions in which each elementary step is irreversible, the rate of the reaction is set by the slowest elementary step (i.e., the rate-limiting step).

Essential knowledge 4.C.3: Reaction intermediates, which are formed during the reaction but not present in the overall reaction, play an important role in multistep reactions.

- a. A reaction intermediate is produced by some elementary steps and consumed by others, such that it is present only while a reaction is occurring.
- b. Experimental detection of a reaction intermediate is a common way to build evidence in support of one reaction mechanism over an alternative mechanism.

4.C Learning Objective:

LO 4.7 The student is able to evaluate alternative explanations, as expressed by reaction mechanisms, to determine which are consistent with data regarding the overall rate of a reaction, and data that can be used to infer the presence of a reaction intermediate. [See SP 6.5, connects to 4.C.1, 4.C.2, 4.C.3]

Enduring understanding 4.D: Reaction rates may be increased by the presence of a catalyst. Essential knowledge 4.D.1: Catalysts function by lowering the activation energy of an elementary step in a reaction mechanism, and by providing a new and faster reaction mechanism.

- a. A catalyst can stabilize a transition state, lowering the activation energy and thus increasing the rate of a reaction.
- b. A catalyst can increase a reaction rate by participating in the formation of a new reaction intermediate, thereby providing a new reaction pathway or mechanism.

4.D.1 Learning Objective:

LO 4.8 The student can translate among reaction energy profile representations, particulate representations, and symbolic representations (chemical equations) of a chemical reaction occurring in the presence and absence of a catalyst. [See SP 1.5]

Essential knowledge 4.D.2: Important classes in catalysis include acid-base catalysis, surface catalysis, and enzyme catalysis.

- a. In acid-base catalysis, a reactant either gains or loses a proton; this changes the rate of the reaction.
- b. In surface catalysis, either a new reaction intermediate is formed, or the probability of successful collisions is modified.
- c. Some enzymes accelerate reactions by binding to the reactants in a way that lowers the activation energy. Other enzymes react with reactant species to form a new reaction intermediate.

4.D.2 Learning Objective:

LO 4.9 The student is able to explain changes in reaction rates arising from the use of acid-base catalysts,

surface catalysts, or enzyme catalysts, including selecting appropriate mechanisms with or without the catalyst present. [See SP 6.2, 7.2]