

CHEMICAL KINETICS

Pg-1

Rate of Reaction :

$$\text{Rate} = \frac{\text{Change in Conc or Pressure}}{\text{Time taken}}$$

$$\text{Unit} \rightarrow \text{mol L}^{-1} \text{T}^{-1} \text{ or atm T}^{-1}$$

* ROR can never be negative. (-ve)

Rate of Reaction. (A \rightarrow B)

Average Rate

$$\text{Rate} = -\frac{\Delta(A)}{\Delta t} = \frac{\Delta B}{\Delta t}$$



$$R_{\text{avg}} = \left(\frac{A_1 - A_2}{t_2 - t_1} \right)$$

Instantaneous Rate

$$\text{Rate} = -\frac{d(A)}{dt} = \frac{d(B)}{dt}$$



$$\text{Rate} = \text{slope} = \left| \frac{d(A)}{dt} \right|$$



$$\text{Rate (ROR)} = -\frac{d(\text{N}_2)}{dt} = -\frac{d(\text{H}_2)}{3dt} = \frac{1}{2} \frac{d(\text{NH}_3)}{dt}$$

$$\text{Rate of Disappearance} = -\frac{d(\text{N}_2)}{dt} = -\frac{d(\text{H}_2)}{dt}$$

$$\text{Rate of Appearance} = \frac{d(\text{NH}_3)}{dt} \text{ (Product)}$$

ROR & RODA does not include the St. Coeff.



$$\text{ROR} = -\frac{\text{RODA}}{a} = \frac{\text{RODB}}{b} = \frac{\text{RODC}}{c} = \frac{\text{RODD}}{d}$$

$$\text{ROR} = -\frac{1}{a} \frac{d(A)}{dt} = -\frac{1}{b} \frac{d(B)}{dt} = \frac{1}{c} \frac{d(C)}{dt} = \frac{1}{d} \frac{d(D)}{dt}$$

~ Differential Rate Law

Q. The rate of the reaction: $2\text{N}_2\text{O}_5 \rightarrow 4\text{NO}_2 + \text{O}_2$
Can be written in three ways \rightarrow

$$-\frac{d(\text{N}_2\text{O}_5)}{dt} = K [\text{N}_2\text{O}_5] ; \frac{d(\text{NO}_2)}{dt} = k' [\text{N}_2\text{O}_5]$$

$$\frac{d(\text{O}_2)}{dt} = K'' [\text{N}_2\text{O}_5]$$

$$\text{Soln. ROR} = -\frac{1}{2} \frac{d(\text{N}_2\text{O}_5)}{dt} = \frac{1}{4} \frac{d(\text{NO}_2)}{dt} = \frac{d(\text{O}_2)}{dt}$$

$$= -\frac{K [\text{N}_2\text{O}_5]}{2} = \frac{K' [\text{N}_2\text{O}_5]}{4} = \frac{K'' [\text{N}_2\text{O}_5]}{1}$$

$$\text{ROR} = K' = 2K \quad K'' = \frac{K}{2}$$

$$Q = 0.3 + \log \left(-\frac{d(A)}{dt} \right) = 0.18 + \log \left(\frac{d(B)}{dt} \right)$$

write the reaction.

$$0.3 + \log \left(-\frac{d(A)}{dt} \right) = 0.18 + \log \left(\frac{d(B)}{dt} \right)$$

$$0.3 + \log \left(-\frac{d(A)}{dt} \right) = 0.18 + \log \left(\frac{d(B)}{dt} \right)$$



Molecularity :

Δ Can be integer (1, 2 or 3) but it cannot be zero, negative or fractional.

Δ For elementary reaction: Molecularity is equal to its order

Δ Maximum value of molecularity is 3. (or order)

Δ For complex rxn molecularity of each step of mechanism is defined separately. \therefore molecularity cannot be defined for whole complex reaction at once.

Δ Molecularity of a reaction may or may not be equal to order of reaction.

Δ Molecularity can not be determined by balanced chemical rxn and can only be determined from simple reaction

Manual Solution Of Chemical Kinetics

Alexander N. Gorban, Iliya V. Karlin



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Solutions Manual: Sm Chemical Kinetics and React Dyn Paul L. Houston, 2001 **Chemical Engineering Kinetics** Joseph Mauck Smith, C. Y. Cha, 1971 *An Introduction to Chemical Engineering Kinetics and Reactor Design* Charles G. Hill, 1977 **Chemical Engineering Kinetics** Joseph Mauk Smith, 1983 *Chemical Kinetics*, **Catalog of Copyright Entries. Third Series** Library of Congress. Copyright Office, 1976 *Physical Chemistry : Solutions Manual* Robert A. Alberty, 1980 **Invariant Manifolds for Physical and Chemical Kinetics** Alexander N. Gorban, Iliya V. Karlin, 2005-02-01 By bringing together various ideas and methods for extracting the slow manifolds the authors show that it is possible to establish a more macroscopic description in nonequilibrium systems The book treats slowness as stability A unifying geometrical viewpoint of the thermodynamics of slow and fast motion enables the development of reduction techniques both analytical and numerical Examples considered in the book range from the Boltzmann kinetic equation and hydrodynamics to the Fokker Planck equations of polymer dynamics and models of chemical kinetics describing oxidation reactions Special chapters are devoted to model reduction in classical statistical dynamics natural selection and exact solutions for slow hydrodynamic manifolds The book will be a major reference source for both theoretical and applied model reduction Intended primarily as a postgraduate level text in nonequilibrium kinetics and model reduction it will also be valuable to PhD students and researchers in applied mathematics physics and various fields of engineering Physical Chemistry Peter Atkins, Julio de Paula, 2002 New edition of the overwhelmingly favorite text for the physical chemistry course

Chemical Kinetics and Dynamics Jeffrey I. Steinfeld, Joseph Salvatore Francisco, William L. Hase, 1999 This text presents a balanced presentation of the macroscopic view of empirical kinetics and the microscopic molecular viewpoint of chemical dynamics This second edition includes the latest information as well as new topics such as heterogeneous reactions in atmospheric chemistry reactant product imaging and molecular dynamics of H₂ *Monthly Catalog of United States Government Publications, Cumulative Index* United States. Superintendent of Documents, 1970 Kinetics of Catalytic Reactions--Solutions Manual M. Albert Vannice, 2008-03-27 This manual of solutions to the problems in Kinetics of Catalytic Reactions has been prepared to assist those who use this book in a teaching function However these solutions should also benefit those outside the classroom who want to apply the principles and concepts that are discussed in the book By studying and observing the approaches used in solving these problems it is very likely that similar applications can be envisioned in different kinetic problems that the investigator might face Thus the availability of these solutions is a good learning tool for everyone Additional details and insight about the solutions provided can be obtained by reading the cited references I have tried to eliminate all errors both conceptual and typographical in these solutions however the probability is high that I have not succeeded completely Should any errors of commission or omission be found I would greatly appreciate being informed I can be reached at this email address mavche engr psu edu or mail can be sent to me at 107 Fenske Laboratory Department

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