Introduction

As a discipline, physical chemistry attempts to understand chemistry, in all its complexity, as a consequence of a few fundamental physical laws. This fascinating enterprise includes chemical processes in physics and biology, as well as engineering. On a deeper level, physical chemistry aims to understand and quantify the tremendous variety that matter takes in our world. The unifying nature of physical chemistry is emphasized in the book by its organization – beginning with atoms and molecules, proceeding to molecular assemblies of increasing complexity, and ending with the emergence of matter that carries information, in other words the origin of life, a physicochemical process of unique importance. The aim is to show the broad scope and coherence of physical chemistry.

The book begins with the most basic and central question in physical chemistry, 'Why do atoms and molecules form from a collection of electrons and nuclei?' The answer to this question requires a fundamentally different way of thinking about the world than we are used to from our daily macroscopic experiences; it requires that the fascinating and strange predictions of quantum mechanics guide us. Thus, Chapter 1 exposes you to some astonishing experimental facts that require this new way of thinking. We show you that the given facts can be seen as consequences of some fundamental postulates. On this basis Chapter 2 explains the existence of the simplest atom (hydrogen atom, H) and the simplest molecule (hydrogen molecule ion, H_2^+) in terms of a simple model of an electron confined to a region of space (particle-in-a-box). Next the book explores the quantum-mechanical basis of chemical bonding (Chapters 3 to 7 and 13) and how we use light to probe molecular structure, a field of study called spectroscopy (Chapters 8 to 12). Throughout these chapters the simple particle-in-a-box model is used as a touchstone to reinforce and develop the understanding of chemical bonding. Although some modern experimental methods can probe the properties of individual atoms and molecules, most experiments are performed with collections of atoms and/or molecules. Chapter 13 provides an introduction and overview of some essential aspects of how to think about such collections. This chapter begins the book's consideration of a second fundamental question in physical chemistry, 'What is the connection between molecular properties and the macroscopic properties of matter?' Chapters 14 through 18 develop our atomistic view of matter and its utility for quantitatively predicting the properties of a large collection of molecules as a function of what is called temperature in the macroscopic description of matter.

In order to present this description most clearly we use simplified models, for example, the Ideal Gas Law, which ignores intermolecular forces. With this fundamental understanding in hand, the book proceeds to develop the macroscopic description of chemical systems with intermolecular forces (Chapters 19 through 21). Chapters 22 and 23 apply these developments to chemical equilibria in aqueous solutions, biosystems, and electrochemistry.

'How do molecules and atoms (reactants) transform into different molecules and atoms (products)?' For many practicing chemists, this question is the essence of chemistry. We consider chemical reaction rates and reaction dynamics in Chapters 24 and 25. Although

Principles of Physical Chemistry, Second Edition, by Hans Kuhn, Horst-Dieter Försterling, and David H. Waldeck.

much progress has been made in providing a quantitatively accurate picture of reaction dynamics, this area remains a current frontier of physical chemistry.

The final chapters of the book address the question 'Why do molecules aggregate into organized assemblies and how does the organization of molecules give rise to new properties?' First we develop some of the primary physicochemical considerations for understanding organized molecular assemblies; in particular, we explore the properties of macromolecules (Chapter 26) and of interfaces (Chapter 27), because they can be used to organize molecules, or molecular subunits, in space. Chapter 28 explores how the organization of functional molecules can be used to create new behaviors that are characteristic of the supramolecular assembly, distinct from the individual molecule behaviors. The understanding of supramolecular machines and organized assemblies is a new frontier in physical chemistry research. The final chapter explores some of the underlying physicochemical principles that are important for evolution and the origin of life.

Although the sequence of chapters in the book need not determine the sequence of topics in a physical chemistry lecture course, the organization of the chapters in the book and its broad scope aim to emphasize the logical progression and unity of physical chemistry. Whatever order of topics is chosen, it is crucial to present the unifying nature of physical chemistry to the student. Where possible, the logical sequence in a given chapter is constructed to evolve from the more basic and simple picture to a more sophisticated treatment for the more experienced students. If such a section is too difficult in a first reading, it is often still possible to skip it and proceed onward to the next chapter without loss of the general picture. Hence, if a section is too difficult to study with excitement, consider skipping it and returning at a later stage.

The book aims to develop one's intuition on how research works by presenting many exciting original ideas and providing instructive examples that inspire thinking. Rather than always aiming for rigor, the discussion uses simplified models and approximations that can develop our intuition and guide our thinking. For these reasons, original research findings and current research findings are included in the examples or as part of problems and exercises to be worked. Lastly, the text is only a tool through which the student must explore and discover the rich field of physical chemistry for her- or himself.