

Words to the reader about how to use this textbook

I. What This Book Does and Does Not Contain

This text is intended for use by beginning graduate students and advanced upper division undergraduate students in all areas of chemistry.

It provides:

- (i) An introduction to the fundamentals of quantum mechanics as they apply to chemistry,
- (ii) Material that provides brief introductions to the subjects of molecular spectroscopy and chemical dynamics,
- (iii) An introduction to computational chemistry applied to the treatment of electronic structures of atoms, molecules, radicals, and ions,
- (iv) A large number of exercises, problems, and detailed solutions.

It does not provide much historical perspective on the development of quantum mechanics. Subjects such as the photoelectric effect, black-body radiation, the dual nature of electrons and photons, and the Davisson and Germer experiments are not even discussed.

To provide a text that students can use to gain introductory level knowledge of quantum mechanics as applied to chemistry problems, such a non-historical approach had to be followed. This text immediately exposes the reader to the machinery of quantum mechanics.

Sections 1 and 2 (i.e., Chapters 1-7), together with Appendices A, B, C and E, could constitute a one-semester course for most first-year Ph. D. programs in the U. S. A. Section 3 (Chapters 8-12) and selected material from other appendices or selections from Section 6 would be appropriate for a second-quarter or second-semester course. Chapters 13- 15 of Sections 4 and 5 would be of use for providing a link to a one-quarter or one-semester class covering molecular spectroscopy. Chapter 16 of Section 5 provides a brief introduction to chemical dynamics that could be used at the beginning of a class on this subject.

There are many quantum chemistry and quantum mechanics textbooks that cover material similar to that contained in Sections 1 and 2; in fact, our treatment of this material is generally briefer and less detailed than one finds in, for example, Quantum Chemistry, H. Eyring, J. Walter, and G. E. Kimball, J. Wiley and Sons, New York, N.Y. (1947), Quantum Chemistry, D. A. McQuarrie, University Science Books, Mill Valley, Ca. (1983), Molecular Quantum Mechanics, P. W. Atkins, Oxford Univ. Press, Oxford, England (1983), or Quantum Chemistry, I. N. Levine, Prentice Hall, Englewood Cliffs,

N. J. (1991), Depending on the backgrounds of the students, our coverage may have to be supplemented in these first two Sections.

By covering this introductory material in less detail, we are able, within the confines of a text that can be used for a one-year or a two-quarter course, to introduce the student to the more modern subjects treated in Sections 3, 5, and 6. Our coverage of modern quantum chemistry methodology is not as detailed as that found in Modern Quantum Chemistry, A. Szabo and N. S. Ostlund, Mc Graw-Hill, New York (1989), which contains little or none of the introductory material of our Sections 1 and 2.

By combining both introductory and modern up-to-date quantum chemistry material in a single book designed to serve as a text for one-quarter, one-semester, two-quarter, or one-year classes for first-year graduate students, we offer a unique product.

It is anticipated that a course dealing with atomic and molecular spectroscopy will follow the student's mastery of the material covered in Sections 1- 4. For this reason, beyond these introductory sections, this text's emphasis is placed on electronic structure applications rather than on vibrational and rotational energy levels, which are traditionally covered in considerable detail in spectroscopy courses.

In brief summary, this book includes the following material: