

Book Review [1]

Fundamentals of Quantum Chemistry: Molecular Spectroscopy and Modern Electronic Structure Computations. By Michael Mueller (Dept. of Chemistry, Rose-Hulman Institute of Technology, Terre Haute, IN, USA). Kluwer Academic/Plenum Publishers: New York. June 2001, Hardbound. 280 pp. EUR 75.75 / USD 69.50 / GBP 48.00. ISBN 0-306-46596-5

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I enjoyed reading this book. The message at the publisher's website [2] gives a very good introduction to this book. I copied and pasted the paragraphs here:

This text is designed as a practical introduction to quantum chemistry. Quantum chemistry is applied to explain and predict molecular spectroscopy and the electronic structure of atoms and molecules. In addition, the text provides a practical guide to using molecular mechanics and electronic structure computations including *ab initio*, semi-empirical, and density functional methods. The use of electronic structure computations is a timely subject as its applications in both theoretical and experimental chemical research is increasingly prevalent.

This text is written in a format that fosters mastery of the subject both in competency in the mathematics and in obtaining a conceptual understanding of quantum mechanics. The chemistry student's interest is maintained early on in the text where quantum mechanics is developed by applying it to molecular spectroscopy and through conceptual questions labeled as Chemical Connection. Questions throughout the text labeled as Chemical Connection and Points of Further Understanding focus on conceptual understanding and consequences of quantum mechanics. If an Instructor chooses, these questions can be used as a basis for classroom discussion encouraging cooperative learning techniques.

This text provides a solid foundation from which students can readily build further knowledge of quantum chemistry in more advanced courses. In cases where this is a final course in quantum chemistry, this text provides the student not only with an appreciation of the importance of quantum mechanics to chemistry, but also with a practical guide to using electronic structure computations.

Contents: Acknowledgements. Foreword. Preface. 1. Classical Mechanics. 2. Fundamentals of Quantum Mechanics. 3. Rotational Motion. 4. Techniques of Approximation. 5. Particles Encountering a Finite Potential Energy. 6. Vibrational/Rotational Spectroscopy of Diatomic Molecules. 7. Vibrational and Rotational Spectroscopy of Polyatomic Molecules. 8. Atomic Structure and Spectra. 9. Methods of Molecular Electronic Structure Computations. Appendices. Index.

Notes

1. *Editor's Note:* The brief summary and the contents of the books are reported as provided by the author or the publishers. Authors and publishers are encouraged to send review copies of their recent books of potential interest to readers of *Entropy* to the Editor-in-Chief (Dr. Shu-Kun Lin, MDPI, Saengergasse 25, CH-4054 Basel, Switzerland. Tel. +41 79 322 3379, Fax +41 61 302 8918, E-mail: lin@mdpi.org). Some books will be offered to the scholarly community for the purpose of preparing full-length reviews.
2. The URL for the book is <http://www.wkap.nl/prod/b/0-306-46596-5>.

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