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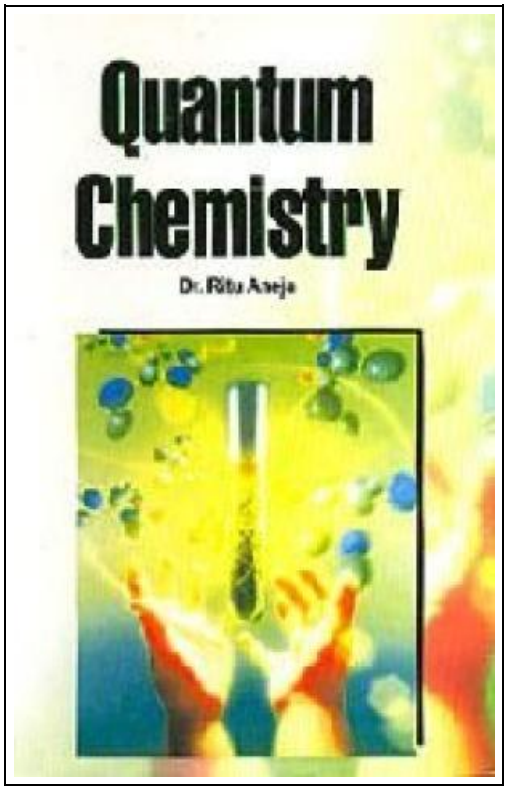


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***(Prof. Antone Olson II)***

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Shree, 2005. Hardcover. Book Condition: New. Contents Preface. 1. Quantum mechanics and their interpretation. 2. Semiempirical methods. 3. Ab Initio molecular dynamics. 4. Ab Initio quantum chemistry. 5. Contextuality. 6. Coordinate systems and transformations. 7. Reciprocity theorems and pseudoelectric fields. 8. Hybrid quantum mechanics/molecular mechanics approaches. 9. Angular momentum theory. 10. Ab Initio treatment of large molecules. 11. Quantum mechanics no hidden variables theorems and physics. 12. Optimal control of quantum systems. Quantum chemistry is the application of quantum mechanics to problems in chemistry. The fundamental methods of quantum chemistry date back to the earliest days of quantum mechanics in the earlier decades of the twentieth century. However widespread quantitative applications have only become common practice in recent times primarily because of the explosive developments in computer hardware and the associated achievements in the design of new and improved theoretical methods and computational techniques. It is highly desirable for students in all areas of chemistry to understand modern methods of electronic structure calculation and this book has been written with this goal in mind. It integrates the fundamentals of quantum theory with a rigorous introduction to quantum chemistry. It would make a good reference tool for a yearlong introduction to quantum mechanics and quantum chemistry for first year graduate students in physical chemistry. 294 pp.

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