<<量子化学>>

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内容概要

a solutions manual for the problems in the book is available.

the expanding role of quantum chemistry makes it highly desirable for students in all areas of chemistry to understand modern methods of electronic structure calcula-tion, and this book has been written with this goal in mind.

i have tried to make explanations clear and complete, without glossing over diffi-cult or subtle points. derivations are given with enough detail to make them easy to fol-low, and i avoid resorting to the frustrating phrase "it can be shown that" wherever possible. the aim is to give students a solid understanding of the physical and mathe-matical aspects of quantum mechanics and molecular electronic structure. the book is designed to be useful to students in all branches of chemistry, not just future quantum chemists. however, the presentation is such that those who do go on in quantum chem-istry will have a good foundation and will not be hampered by misconceptions.

an obstacle faced by many chemistry students in learning quantum mechanics is their unfamiliarity with much of the required mathematics. in this text i have included detailed treatments of operators, differential equations, simultaneous linear equations,and other needed topics. rather than putting all the mathematics in an introductory chapter or a series of appendices, i have integrated the mathematics with the physics and chemistry. immediate application of the mathematics to solving a quantum-mechanical problem will make the mathematics more meaningful to students than would separate study of the mathematics. i have also kept in mind the limited physics background of many chemistry students by reviewing topics in physics.

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书籍目录

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编辑推荐

《量子化学(第6版)》共18章，总共750多页，内容非常丰富。
书中把量子力学的基本原理，各个不同体系中薛定谔方程及其近似解法，尤其针对化学特有的分子体系的量子力学理论与电子结构计算方法（从头算、密度函数、半经验、分子力学、价键理论）进行了详细介绍，并针对上述方法在计算基态分子性质的性能方面进行了十分详细的对比分析，对实际应用有很好的参考价值。

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