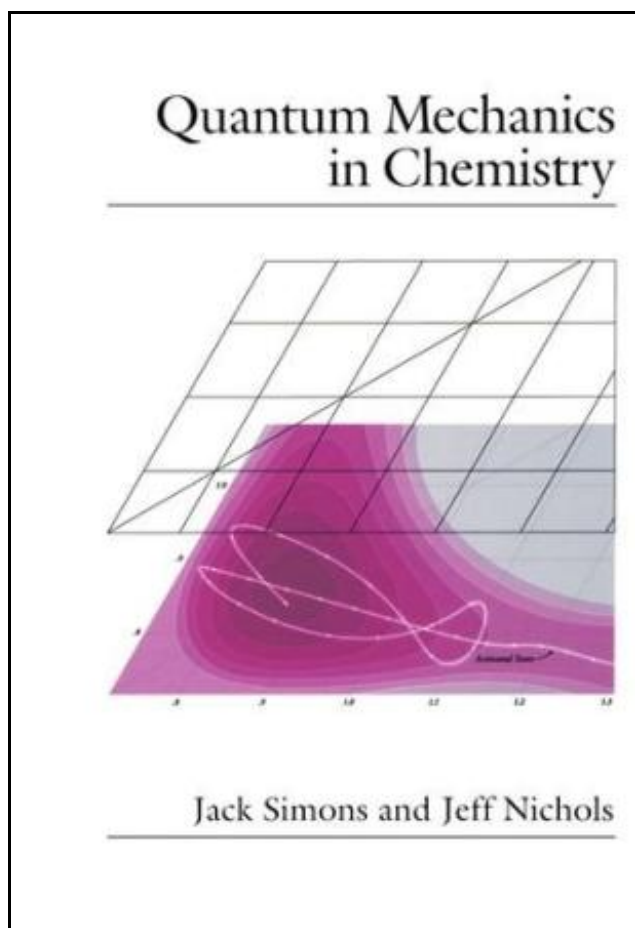# Quantum Mechanics in Chemistry (Topics in Physical Chemistry)

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QUANTUM MECHANICS IN CHEMISTRY (TOPICS IN PHYSICAL CHEMISTRY)

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Oxford University Press, 1997. Book Condition: New. Brand New, Unread Copy in Perfect Condition. A+ Customer Service! Summary: Section 1 The Basic Tools of Quantum Mechanics1. Quantum Mechanics describes matter in terms of wavefunctions and energy levels. Physical measurements are described in terms of operators acting on wavefunctions.I. Operators, Wavefunctions, and the Schrodinger EquationII. Examples of Solving the Schrodinger EquationIII. The Physical Relevance of Wavefunctions, Operators, and Eigenvalues2. Approximation methods can be used when exact solutions to the Schrodinger equation can not be found.I. The Variational MethodII. Perturbation TheoryIII. Example Applications of Variational and Perturbation Methods3. The Application of the Schrodinger equation to the motions of electrons and nuclei in a molecule lead to the chemists'' picture of electronic energy surfaces on which vibration and rotation occurs and among which transitions take place.I. The Born-Oppenheimer Separation of Electronic and Nuclear MotionsII. Rotation and Vibration of Diatomic MoleculesIII. Rotation of Polyatomic MoleculesIV. SummarySummarySection 1 Exercises and Problems and SolutionsSection 2 Simple Molecular Orbital Theory4. Valence atomic orbitals on neighboring atoms combine to form bonding, non-bonding, and antibonding molecular orbitals.I. Atomic OrbitalsII. Molecular Orbitals5. Molecular orbitals possess specific topology, symmetry, and energy-level patterns.I. Orbital Interaction TopologyII. Orbital Symmetry6. Along "reaction paths", orbitals can be connected one-to-one according to their symmetries and energies. This is the origin of the Woodward-Hoffman rules.I. Reduction in Symmetry Along Reaction PathsII. Orbital Correlation Diagrams - Origins of the Woodward-Hoffman Rules7. The most elementary molecular orbital models contain symmetry, nodal pattern, and approximate energy information.I. The LCAO-MO Expansion and the Orbital-Level Schrodinger EquationII. Determining the Effective Potential VSection 2 Exercises and Problems and SolutionsSection 3 Electronic Configurations, Term Symbols, and States8. Electrons are placed into orbital to form configurations, each of which can be labeled by its symmetry. The configurations may "interact" strongly if they have similar energies....

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