This is a text dealing with the basics of quantum mechanics and electronic structure theory. It provides an introduction to molecular spectroscopy and to the subject of molecular dynamics.

• Front Matter

• 1: The Basic Tools of Quantum Mechanics

\[ E_n^{(1)} = \langle \phi_n | H_1 | \phi_n \rangle \]
\[ c_{nk}^{(1)} = \frac{\langle \phi_k | H_1 | \phi_n \rangle}{E_n^{(0)} - E_k^{(0)}} \]
\[ E_n^{(2)} = \sum_{k \neq n} \frac{|\langle \phi_k | H_1 | \phi_n \rangle|^2}{E_n^{(0)} - E_k^{(0)}} \]

• 2: Approximation Methods

• 3: Nuclear Motion
4: Atomic Orbitals

5: Molecular Orbitals

6: Quantum Mechanics in Reactions

7: Further Characterization of Molecular Orbitals
8: Electronic Configurations

$$\mathbf{B} = \begin{pmatrix}
B_{1,1} & B_{1,2} & \cdots & B_{1,N} \\
B_{2,1} & B_{2,2} & \cdots & B_{2,N} \\
\vdots & \vdots & \ddots & \vdots \\
B_{N,1} & B_{N,2} & \cdots & B_{N,N}
\end{pmatrix}. $$

9: Symmetry of Electronic Wavefunctions

- 10: Angular Momentum and Group Symmetries of Electronic Wavefunctions

$$\langle \Psi | \hat{F} | \Psi \rangle = \sum_{i=1}^{N} \langle \phi_{i} | \hat{f} | \phi_{i} \rangle,$$

$$\langle \Psi | \hat{F} | \Psi_{m}^{p} \rangle = \langle \phi_{m} | \hat{f} | \phi_{p} \rangle,$$

$$\langle \Psi | \hat{F} | \Psi_{ran}^{p} \rangle = 0.$$

11: Evaluating the Matrix Elements of N-electron Wavefunctions

$$\begin{array}{c}
\text{A} \text{B} \quad \text{A}^{+} + \text{B}^{-} \\
\text{A} \text{B} \quad \text{A}^{-} + \text{B}^{+} \\
\text{A} \text{B} \quad \text{A}^{*} + \text{B}^{*}
\end{array}$$
12: Quantum Mechanical Picture of Bond Making and Breaking Reactions

13: Molecular Rotation and Vibration

14: Time-dependent Quantum Dynamics

15: Spectroscopy

16: Collisions and Scattering
17: Higher Order Corrections to Electronic Structure

18: Multiconfiguration Wavefunctions

19: Multi-Determinant Wavefunctions

20: Response Theory

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21: Problem Sets
Contributors and Attributions

- Jack Simons (Henry Eyring Scientist and Professor of Chemistry, U. Utah) Telluride Schools on Theoretical Chemistry and Jeff A. Nichols (Oak Ridge National Laboratory)