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.

• 1: The Basic Tools of Quantum Mechanics

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

• 2: Approximation Methods

• 3: Nuclear Motion

• 4: Atomic Orbitals
5: Molecular Orbitals

constructive orbital overlap

6: Quantum Mechanics in Reactions

7: Further Characterization of Molecular Orbitals

8: Electronic Configurations

$$B = \begin{pmatrix}
B_{1,1} & B_{1,2} & \cdots & B_{1,N} \\
B_{2,1} & B_{2,2} & \cdots & B_{2,N} \\
\vdots & \vdots & \ddots & \vdots \\
B_{N,1} & B_{N,2} & \cdots & B_{N,N}
\end{pmatrix}$$
9: Symmetry of Electronic Wavefunctions

- 10: Angular Momentum and Group Symmetries of Electronic Wavefunctions

\[ \langle \Psi | \hat{F} | \Psi \rangle = \sum_{i=1}^{N} \langle \phi_i | \hat{F} | \phi_i \rangle, \]
\[ \langle \Psi | \hat{F} | \Psi_{m}^{p} \rangle = \langle \phi_m | \hat{F} | \phi_p \rangle, \]
\[ \langle \Psi | \hat{F} | \Psi_{ran}^{ran} \rangle = 0. \]

- 11: Evaluating the Matrix Elements of N-electron Wavefunctions

- 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

No image available

21: Problem Sets

22: Problems
Contributors

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