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

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

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

\[ \langle \Psi | \hat{F}^\dagger | \Psi \rangle = \sum_{i=1}^{N} \langle \phi_i | \hat{f}^\dagger | \phi_i \rangle, \]

\[ \langle \Psi | \hat{F}^\dagger | \Psi_m^p \rangle = \langle \phi_m | \hat{f}^\dagger | \phi_p \rangle, \]

\[ \langle \Psi | \hat{F}^\dagger | \Psi_{ran} \rangle = 0. \]

11: Evaluating the Matrix Elements of N-electron Wavefunctions

\[ \mathbf{A} \rightarrow \mathbf{B} \rightarrow \mathbf{A}^\oplus + \mathbf{B}^\ominus \]

\[ \mathbf{A} \rightarrow \mathbf{B} \rightarrow \mathbf{A}^\ominus + \mathbf{B}^\oplus \]

\[ \mathbf{A} \rightarrow \mathbf{B} \rightarrow \mathbf{A}^\ast + \mathbf{B}^\ast \]
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

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• 18: Multiconfiguration Wavefunctions

![Diagram]

• 19: Multi-Determinant Wavefunctions

![Diagram]

• 20: Response Theory

![Diagram]

• No image available

21: Problem Sets
Contributors and Attributions

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