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

\[ E_{n}^{(1)} = \langle \phi_{n} \mid H_{1} \mid \phi_{n} \rangle \]

\[ c_{nk}^{(1)} = \frac{\langle \phi_{k} \mid H_{1} \mid \phi_{n} \rangle}{E_{n}^{(0)} - E_{k}^{(0)}} \]

\[ E_{n}^{(2)} = \sum_{k \neq n} \frac{|\langle \phi_{k} \mid H_{1} \mid \phi_{n} \rangle|^{2}}{E_{n}^{(0)} - E_{k}^{(0)}} \]

2: Approximation Methods

3: Nuclear Motion
4: Atomic Orbitals

5: Molecular Orbitals

6: Quantum Mechanics in Reactions

7: Further Characterization of Molecular Orbitals

constructive orbital overlap
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

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

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

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

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

A – B → A⁺ + B⁻

A – B → A⁻ + B⁺

A – B → A⁺ + B⁺
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

21: Problem Sets
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