Molecular vibrations and chemical reaction dynamics (KDIT73)

topics

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1. The Born-Oppenheimer approximation
2. Fundamentals of variational and perturbation methods
3. Potential energy surfaces
4. Variational solution of the vibrational-rotational Schrödinger equation
   - Coordinates
   - Operators (*kinetic and potential energy*)
   - Basis functions
   - Matrix representation (*finite basis representation (FBR), discrete variable representation (DVR), variational basis representation (VBR)*)
   - Diagonalization of the Hamiltonian matrix
5. Diatomic molecules (*a vibrational-rotational DVR code step by step*)
6. Reaction dynamics
   - The quasi-classical trajectory (QCT) method
   - Initial conditions
   - Product analysis (*standard methods and new developments (1GB)*)
   - The zero-point energy problem in classical dynamics (*active and passive constraints*)
   - Applications (*mode-selective chemistry*)