**Computational Chemistry**

Errol G. Lewars, Computational Chemistry, Springer, (2011).

Christopher J. Cramer, Essentials of Computational Chemistry, John Wiley & Sons Ltd, (2004).

Chapter 1

**An Outline of What Computational Chemistry Is All About**

1. What You Can Do with Computational Chemistry
2. The Tools of Computational Chemistry

Chapter 2

**The Concept of the Potential Energy Surface**

1. Perspective
2. Stationary Points
3. The Born–Oppenheimer Approximation
4. Geometry Optimization
5. Stationary Points and Normal-Mode Vibrations – Zero Point Energy

Chapter 3

**Molecular Mechanics**

1. Perspective
2. The Basic Principles of Molecular Mechanics

Developing a Forceﬁeld

Parameterizing a Forceﬁeld

A Calculation Using Our Forceﬁeld

1. Examples of the Use of Molecular Mechanics

To Obtain Reasonable Input Geometries for Lengthier (Ab Initio, Semiempirical or Density Functional) Kinds of Calculations

To Obtain Good Geometries (and Perhaps Energies) for Small- to Medium-Sized Molecules

To Calculate the Geometries and Energies of Very Large Molecules, Usually Polymeric Biomolecules (Proteins and Nucleic Acids)

To Generate the Potential Energy Function Under Which Molecules Move, for Molecular Dynamics or Monte Carlo Calculations

As a (Usually Quick) Guide to the Feasibility of, or Likely Outcome of, Reactions in Organic Synthesis

1. Geometries Calculated by MM
2. Frequencies and Vibrational Spectra Calculated by MM
3. Strengths and Weaknesses of Molecular Mechanics

Strengths

Weaknesses

Chapter 4

**Simulations of Molecular Ensembles**

1. Relationship Between MM Optima and Real Systems
2. Phase Space and Trajectories

Properties as Ensemble Averages

Properties as Time Averages of Trajectories

1. Molecular Dynamics

Harmonic Oscillator Trajectories

Non-analytical Systems

Practical Issues in Propagation

Stochastic Dynamics

1. Monte Carlo

Manipulation of Phase-space Integrals

Metropolis Sampling

1. Ensemble and Dynamical Property Examples
2. Key Details in Formalism

Cutoffs and Boundary Conditions

Polarization

Control of System Variables

Simulation Convergence

The Multiple Minima Problem

1. Force Field Performance in Simulations
2. Case Study: Silica Sodalite

Chapter 5

**Ab initio Calculations**

1. Perspective
2. The Basic Principles of the Ab initio Method

Preliminaries

The Hartree SCF Method

The Hartree–Fock Equations

1. Basis Sets

Introduction

Gaussian Functions; Basis Set Preliminaries; Direct SCF

Types of Basis Sets and Their Uses

1. Post-Hartree–Fock Calculations: Electron Correlation

Electron Correlation

The Møller–Plesset Approach to Electron Correlation

The Conﬁguration Interaction Approach to Electron Correlation – The Coupled Cluster Method

1. Applications of the Ab initio Method

Geometries

Energies

Frequencies and Vibrational Spectra

Properties Arising from Electron Distribution: Dipole Moments, Charges, Bond Orders, Electrostatic Potentials, Atoms-in-Molecules (AIM)

Miscellaneous Properties – UV and NMR Spectra, Ionization Energies, and Electron Afﬁnities

Visualization

1. Strengths and Weaknesses of Ab initio Calculations

Strengths

Weaknesses

Chapter 6

**Semiempirical Calculations**

1. Perspective
2. The Basic Principles of SCF Semiempirical Methods

Preliminaries

The Pariser-Parr-Pople (PPP) Method

The Complete Neglect of Differential Overlap (CNDO) Method

The Intermediate Neglect of Differential Overlap (INDO) Method

The Neglect of Diatomic Differential Overlap (NDDO) Methods

1. Applications of Semiempirical Methods

Geometries

Energies

Frequencies and Vibrational Spectra

Properties Arising from Electron Distribution: Dipole Moments, Charges, Bond Orders

Miscellaneous Properties – UV Spectra, Ionization Energies, and Electron Afﬁnities

Visualization

Some General Remarks

1. Strengths and Weaknesses of Semiempirical Methods

Strengths

Weaknesses.

Chapter 7

**Density Functional Calculations**

1. Perspective
2. The Basic Principles of Density Functional Theory

Preliminaries

Forerunners to Current DFT Methods

Current DFT Methods: The Kohn–Sham Approach

1. Applications of Density Functional Theory

Geometries

Energies

Frequencies and Vibrational Spectra

Properties Arising from Electron Distribution – Dipole Moments, Charges, Bond Orders, Atoms-in-Molecules

Miscellaneous Properties – UV and NMR Spectra, Ionization Energies and Electron Afﬁnities, Electronegativity, Hardness, Softness and the Fukui Function

Visualization

1. Strengths and Weaknesses of DFT

Strengths

Weaknesses