

Contents

Part 1. Description of a Chemical System as a Set of m Fixed Nuclei and n Electrons

1.1	Introduction	1
1.2	The SCF-LCAO-MO Approximation	2
1.3	The Correlation Energy Correction	5
1.4	Statistical Estimate of the Correlation Energy	7
1.5	Configuration Interaction	8
1.6	Combination of Statistical Methods and C.I. Techniques	10
1.7	Molecular Extra Correlation Energy	13
1.8	Choice of the Basis Set for the SCF-LCAO-MO Functions	15
1.9	Electron Population Analyses	22
1.10	Bond Energy Analyses in a Single Molecule	28
1.11	Bond Energy Analyses for Molecular Complexes	39
1.12	Bond Energy Analyses to Derive Chemical Structural Formulas	45
1.13	References	57

Part 2. Structure of Liquid Water as a Test Case

2.1	Introduction	60
2.2	Approximate Hartree-Fock Potential for the Water Dimer	60
2.3	Polymers of Water Molecules in the Hartree-Fock Approximation	63
2.4	Monte Carlo Simulation of Liquid Water Using an Hartree-Fock Potential	74
2.5	Structure of Liquid Water Using an Accurate Potential	79
2.6	References	88

Part 3. Coordination Numbers and Solvation Shells

3.1	Introduction	89
3.2	Structure of Water Arounds Ion Pairs	
3.3	The Three-body Effects	98
3.4	More Accurate Determination of the Coordination Numbers for Ions	102

3.5	Solvation Potentials for Amino Acids	103
3.6	Conclusions	106
3.7	References	107