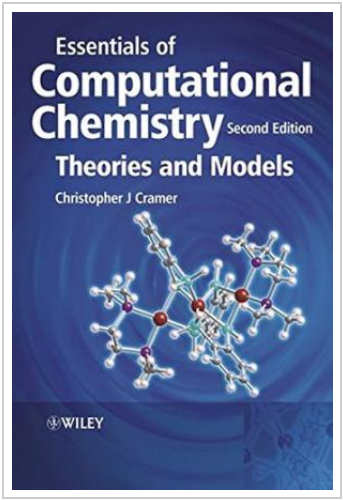

Essentials of Computational Chemistry: Theories and Models

By Cramer, Christopher J.

Wiley, 2004. Book Condition: New. Brand New, Unread Copy in Perfect Condition. A+ Customer Service! Summary: Preface to the First Edition. Preface to the Second Edition. Acknowledgments. 1. What are Theory, Computation, and Modeling? 1.1 Definition of Terms. 1.2 Quantum Mechanics. 1.3 Computable Quantities. 1.3.1 Structure. 1.3.2 Potential Energy Surfaces. 1.3.3 Chemical Properties. 1.4 Cost and Efficiency. 1.4.1 Intrinsic Value. 1.4.2 Hardware and Software. 1.4.3 Algorithms. 1.5 Note on Units. Bibliography and Suggested Additional Reading. References. 2. Molecular Mechanics. 2.1 History and Fundamental Assumptions. 2.2 Potential Energy Functional Forms. 2.2.1 Bond Stretching. 2.2.2 Valence Angle Bending. 2.2.3 Torsions. 2.2.4 van der Waals Interactions. 2.2.5 Electrostatic Interactions. 2.2.6 Cross Terms and Additional Non-bonded Terms. 2.2.7 Parameterization Strategies. 2.3 Force-field Energies and Thermodynamics. 2.4 Geometry Optimization. 2.4.1 Optimization Algorithms. 2.4.2 Optimization Aspects Specific to Force Fields. 2.5 Menagerie of Modern Force Fields. 2.5.1 Available Force Fields. 2.5.2 Validation. 2.6 Force Fields and Docking. 2.7 Case Study: (2R*,4S*)-1-Hydroxy-2,4-dimethylhex-5-ene. Bibliography and Suggested Additional Reading. References. 3. Simulations of Molecular Ensembles. 3.1 Relationship Between MM Optima and Real Systems. 3.2 Phase Space and Trajectories. 3.2.1 Properties as Ensemble Averages. 3.2.2 Properties as Time Averages of Trajectories. 3.3 Molecular Dynamics. 3.3.1 Harmonic Oscillator Trajectories. 3.3.2 Non-analytical...

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