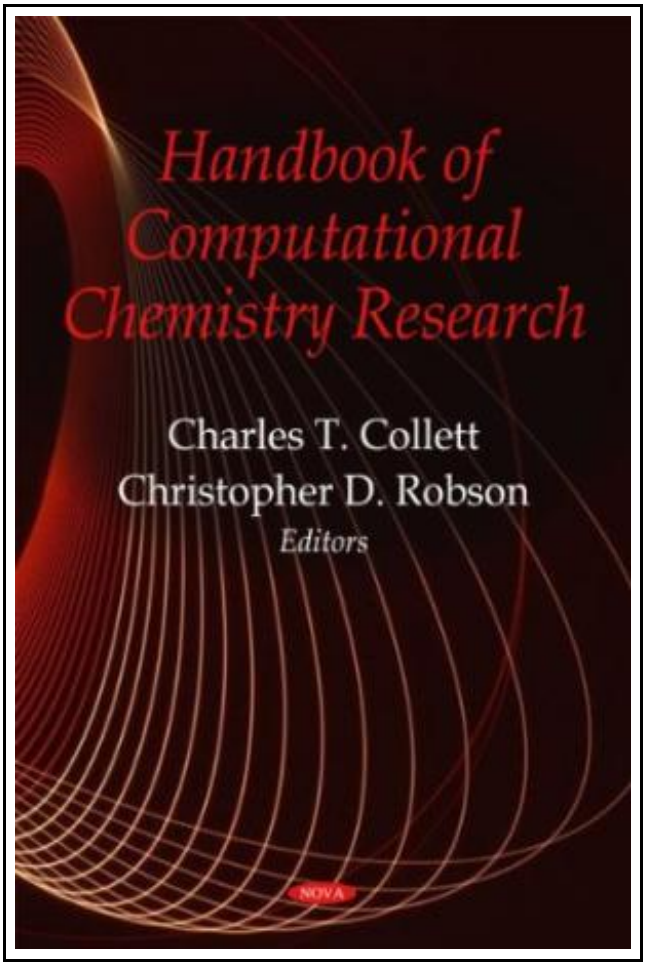
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Nova Science Publishers Inc. Hardback. Book Condition: new. BRAND NEW, Handbook of Computational Chemistry Research, Charles T. Collett, Christopher D. Robson, This book presents ways in which computers can be used to solve chemical problems. One approach develops synoptic algebraic scaling laws to use in place of the case-by-case numerical integrations prescribed by traditional quantum chemistry. The ONIUM hybrid method combines a quantum mechanical method with the molecular mechanical method. One study includes placing functional constraints and testing the performance of the resulting constrained functionals for several chemical properties. A review of the known approximations for the temperature integral is included. Some of the other areas of research discussed include protein coarse-grain models, a specific application of spherical harmonics, use of the FERMO concept to better explain reactions that are HOMO driven, wavelet based approaches and high resolution methods with successful application to a fixed-bed adsorption column model. There is a discussion of stability and thermodynamics, as well as kinetic properties of heterophosphetes and phosphole oxides. A model is proposed that applies methods and concepts in mathematical morphology paradigms to solve the problem of offset curves as well as a description of the solvent effects through the in silico procedures by the use of continuum and discrete models. A simulation method attempts to relate the microscopic details of a system to macroscopic properties of experimental interest. Techniques to retain the use of simple potential functions are also discussed, but with the possibility of allowing them to readjust their properties to fit the potential energy curves of the more complex functions. The Chapman-Cruzen mechanism is also studied using the ideas of the theory of dynamical systems.

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