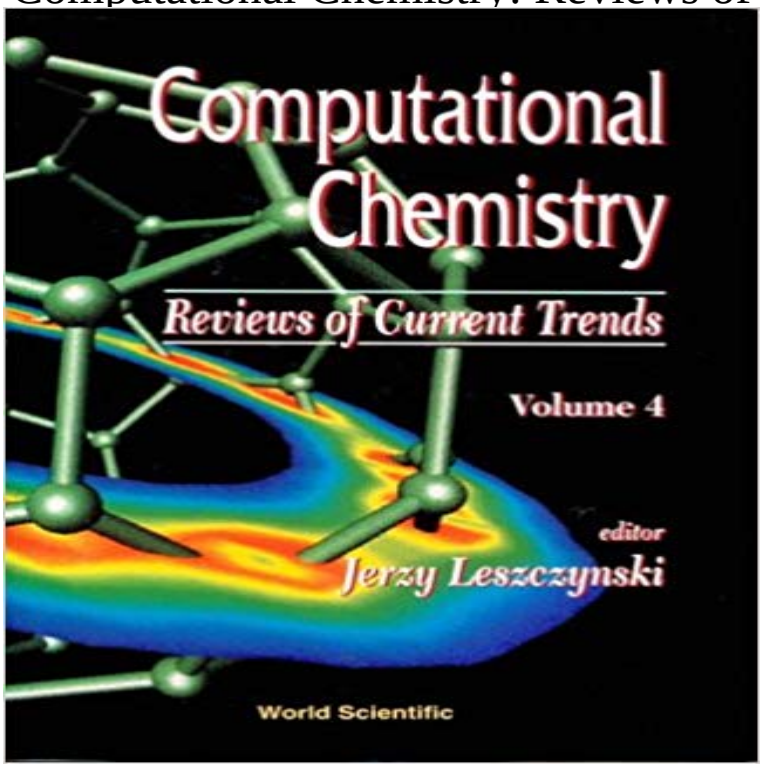
Computational Chemistry: Reviews of Current Trends, Vol. 4



This volume presents a balanced blend of methodological and applied contributions. It supplements well the first three volumes of the series, revealing results of current research in computational chemistry. It also reviews the topographical features of several molecular scalar fields. A brief discussion of topographical concepts is followed by examples of their application to several branches of chemistry.The size of a basis set applied in a calculation determines the amount of computer resources necessary for a particular task. The details of a common strategy the ab initio model potential method which could be used to minimize such a task are revealed in the subsequent contribution. Such an approach is applied to atoms, molecules and solids. Two chapters are devoted to the prediction of solvent effects in biological systems. These effects are significant for interactions of nucleic acid bases and crucial for an evaluation of the free energies that govern the associations of macromolecules in aqueous solutions.A chapter on the developments and applications of the multireference Moller-Plesset method could be used as a reference in theoretical studies of systems where both the dynamical and nondynamical correlation effects should be accounted for. This technique is an efficient tool in such investigations. An explosive application of computational techniques studies of detonation initiation and sensitivity in energetic compounds is discussed in detail in the last chapter. The computational treatment of such unstable compounds allows the prediction of their crucial properties without being subject to their destructive forces.

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