Molecular Electrostatic Potentials: Concepts and Applications (Theoretical and Computational Chemistry)

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Over the past 25 years, the molecular electrostatic potential has become firmly established as an effective guide to molecular interactions. With the recent advances in computational technology, it is currently being applied to a variety of important chemical and biological systems. Its range of applicability has expanded from primarily a focus on sites for electrophilic and nucleophilic attack to now include solvent effects, studies of zeolite, molecular cluster and crystal behavior, and the correlation and prediction of a wide range of macroscopic properties. Moreover, the increasing prominence of density functional theory has raised the molecular electrostatic potential to a new stature on a more fundamental conceptual level. It is rigorously defined in terms of the electron density, and has very interesting topological characteristics since it explicitly reflects opposing contributions from the nuclei and the electrons.

This volume opens with a survey chapter by one of the original pioneers of the use of the electrostatic potential in studies of chemical reactivity, Jacopo Tomasi. Though the flow of the succeeding chapters is not stringently defined, the overall trend is that the emphasis changes gradually from methodology to applications. Chapters discussing more theoretical topics are placed near the end. Readers will find the wide variety of topics provided by an international group of authors both convincing and useful.

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