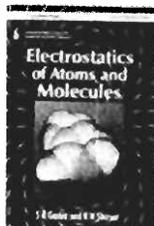


Electrostatics of Atoms and Molecules

G Narahari Sastry



Electrostatics of Atoms and Molecules

S R Gadre and R N Shirsat

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In the last decade or so, in silico prediction of molecular properties have become economic means of achieving quick insights, and in some instances attractive alternatives to the experimental techniques. Modeling the drug-receptor and supramolecular interactions is one of the formidable challenges to modern computational approaches. Collaborative efforts among the biologists, physicists and chemists are essential in understanding the interactions between molecules, particularly biomolecules. Electrostatic interactions are the major contributors along with the van der Waals and dispersive interactions. The book, under review, is divided into four chapters and supplemented by seven appendices. The first chapter makes an unassuming beginning and gives a nice historical introduction along with the basic concepts. The second chapter deals with the experimental and theoretical techniques to obtain the molecular electrostatic potential (MESP), and beautifully illustrates the maps with the graphic visualization programs. Chapter 3 provides some general results followed by

some illustrative applications of MESP in diverse areas. I found that the monograph maintains a fine balance between rigor and application and gives a good exposition to the field of electrostatics and their utility in getting insights in diverse areas. The conventional quantum chemistry textbooks often truncate the treatment of electrostatics in general, and I do not find any other book of Indian origin on this topic at the same level. Thus, it would not be an exaggeration to state that this is the first attempt at a textbook or a monograph which thoroughly discusses the topic of electrostatics in our country.

The other nice feature of the book is the effective utilization of the appendix section. Quite a number of topics, which are of relevance, are dealt in more detail in the appendices, which should be particularly useful to the non-specialists and students. Appendix A, which gives some biographical notes of pioneering contributors in the field, makes interesting reading to everyone. This monograph could have had some more examples on the application of electrostatics in drug design, and docking studies. Obviously, it is impossible to cover all the fundamentals and applications of electrostatics for a book of this size. Thus, this book will be quite useful in providing the correct direction to anybody trying to apply electrostatics to solve structural, mechanistic and reactivity problems in chemistry and biology. The encouraging point in this monograph is that, this would be of interest

to people from various disciplines, such as physics, chemistry, biology, material science, etc. The students and teachers who are working in the areas of computational chemistry, molecular modeling or X-ray crystallography should definitely benefit from this book.

In conclusion, the efforts taken by the authors Gadre and Shirsat in bringing out a reasonably priced monograph on a topic of current

interest are highly commendable. I recommend this book to all the physics, chemistry and biology students who have a keen interest in research as well as to fresh researchers and teachers.

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