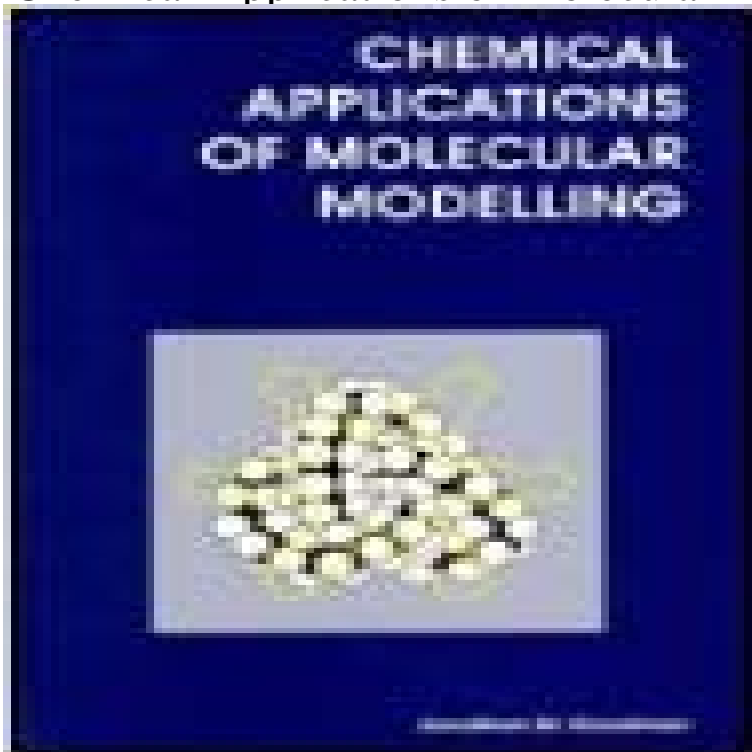


Chemical Applications of Molecular Modelling



As computers become an important part of everyday life, molecular modelling is affecting all parts of chemistry, and is particularly useful in organic chemistry. But how does it work? How reliable is it? What are its limitations? Is it useful for normal chemists? In answering these questions, this book demystifies molecular modelling, enabling the non-specialist to appreciate the power, but also the limitations, of the computational tools available. Chemical Applications of Molecular Modelling provides a background to the methods used and describes how they have developed. It also shows how molecular modelling has been used to address chemical questions commonly asked by the experimental chemist, and includes many examples and case studies. It will be suitable as an undergraduate coursebook - putting normal chemistry course work into perspective with respect to modelling methods - as well as providing a useful reference for researchers. A discussion area and enhanced images from the book are available at: <http://www.chemsoc.org/chembytes/publications/goodman/goodman.htm>

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