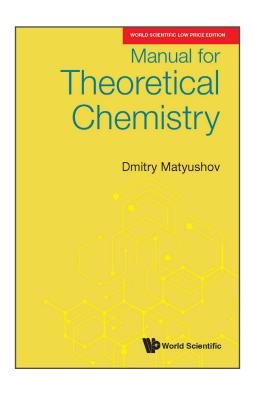




## MANUAL FOR THEORETICAL CHEMISTRY

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USA)



ISBN 9781944660024 Extent: 372pp, PB Pub Date: 2022 Price: Rs. 1195

te: 2022 This study guide aims at explaining theoretical concepts encountered by

ABOUT THE BOOK

practitioners applying theory to molecular science. This is a collection of short chapters, a manual, attempting to walk the reader through two types of topics: (i) those that are usually covered by standard texts but are difficult to grasp and (ii) topics not usually covered, but are essential for successful theoretical research. The main focus is on the latter. The philosophy of this book is not to cover a complete theory, but instead to provide a set of simple study cases helping to illustrate main concepts. The focus is on simplicity. Each section is made deliberately short, to enable the reader to easily grasp the contents. Sections are collated in themed chapters, and the advantage is that each section can be studied separately, as an introduction to more in-depth studies. Topics covered are related to elasticity, electrostatics, molecular dynamics and molecular spectroscopy, which form the foundation for many presently active research areas such as molecular biophysics and soft matter physics. The notes provide a uniform approach to all these areas, helping the reader to grasp the basic concepts from a common set of theoretical tools.

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## READERSHIP

Advanced undergraduate students, graduate students and researchers working in areas of theoretical chemistry, molecular biophysics, and soft matter physics.

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