



The Theory of Intermolecular Forces (Hardback)

By Anthony J Stone

Oxford University Press, United Kingdom, 2013. Hardback. Book Condition: New. 2nd Revised edition. 248 x 176 mm. Language: English . Brand New Book. The theory of intermolecular forces has advanced very greatly in recent years. It has become possible to carry out accurate calculations of intermolecular forces for molecules of useful size, and to apply the results to important practical applications such as understanding protein structure and function, and predicting the structures of molecular crystals. The Theory of Intermolecular Forces sets out the mathematical techniques that are needed to describe and calculate intermolecular interactions and to handle the more elaborate mathematical models. It describes the methods that are used to calculate them, including recent developments in the use of density functional theory and symmetry-adapted perturbation theory. The use of higher-rank multipole moments to describe electrostatic interactions is explained in both Cartesian and spherical tensor formalism, and methods that avoid the multipole expansion are also discussed. Modern ab initio perturbation theory methods for the calculation of intermolecular interactions are discussed in detail, and methods for calculating properties of molecular clusters and condensed matter for comparison with experiment are surveyed.



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Reviews

This book is definitely worth acquiring. I have go through and so i am certain that i will likely to read through again again in the future. Its been printed in an exceptionally basic way in fact it is only after i finished reading this publication in which actually altered me, change the way in my opinion.

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